Euler-Maclaurin expansions without analytic derivatives

Bengt Fornberg *
Department of Applied Mathematics, University of Colorado, Boulder, CO 80309, USA

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Abstract

The Euler-Maclaurin formulas relate sums and integrals. Discovered nearly 300 years ago, they have lost none of their importance over the years, and are nowadays routinely taught in scientific computing and numerical analysis courses. The two common versions can be viewed as providing error expansions for the trapezoidal rule and for the midpoint rule, respectively. More importantly, they provide a means for evaluating many infinite sums to high levels of accuracy. However, in all but the simplest cases, calculating very high order derivatives analytically becomes prohibitively complicated. When approximating such derivatives with finite differences (FD), the choice of step size typically requires a severe trade-off between errors due to truncation and to rounding. We show here that, in the special case of Euler-Maclaurin expansions, FD approximations can provide excellent accuracy without the step size having to go to zero. While FD approximations of low order derivatives to high orders of accuracy have many applications for solving ODEs and PDEs, the present context is unusual in that it relies on FD approximations to derivatives of very high orders. The application to infinite sums ensures that one can use centered FD formulas (which are not subject to the Runge phenomenon).

1 Introduction

The two common versions of the Euler-Maclaurin formula can be seen as error expansions of the trapezoidal rule and the midpoint rule, respectively. In the case of a semi-infinite interval $[x_0, \infty]$, with nodes at $x_k = x_0 + kh$ and at $\xi_k = x_0 + (k + \frac{1}{2})h$, $k = 0, 1, 2, \ldots$, these are[1]:

$$\int_{x_0}^{\infty} f(x)dx - h\sum_{k=0}^{\infty} f(x_k) \approx$$
$$-\frac{h}{2}f(x_0) + \frac{h^2}{12}f^{(1)}(x_0) - \frac{h^4}{720}f^{(3)}(x_0) + \frac{h^6}{30240}f^{(5)}(x_0) - \frac{h^8}{1209600}f^{(7)}(x_0) + - \ldots \,, \tag{1}$$

* *Email*: fornberg@colorado.edu
[1] The coefficients are expressible in terms of Bernoulli numbers; cf. Appendix A.

and

$$\int_{x_0}^{\infty} f(x)dx - h\sum_{k=0}^{\infty} f(\xi_k) \approx$$
$$-\frac{h^2}{24}f^{(1)}(x_0) + \frac{7\,h^4}{5760}f^{(3)}(x_0) - \frac{31\,h^6}{967680}f^{(5)}(x_0) + \frac{127\,h^8}{154828800}f^{(7)}(x_0) + - \ldots\ , \qquad (2)$$

respectively. One use of these expansions (which we denote EM1 and EM2) is to approximate infinite (non-oscillatory) sums in cases where the function can be analytically integrated and also repeatedly differentiated.[2] In case of finite intervals, the expansions can be applied separately at the two ends. An alternate usage is then to approximate integrals by means of finite sums. The two circumstances that makes us focus on the evaluation of infinite sums are:

i. The application to infinite sums ensures that one can use centered FD approximations (rather than much less accurate one-sided ones), and

ii. The decay rate of the expansion coefficients in (1) and (2) turns out to be just fast enough to off-set the danger of using FD approximations for increasingly high order derivatives.

For a brief historical background to this pioneering discovery by Euler and Maclaurin, we quote verbatim the following passage from [24]:

> Maclaurin asked for, and obtained, Stirling's help and criticisms, while his *Treatise of Fluxions* was in proof. This had an interesting sequel. About 1736, Euler wrote to Stirling a letter (now lost) in which he communicated his *Summation Formula.* Stirling in his reply recognized its importance, and that it included his own theorem on $\log n!$ as a particular case, but "warned" Euler that he had read the *identical* theorem in the *Fluxions.* Euler in a long reply, full of interesting mathematical information, waived his claims to priority before Maclaurin. On the whole, Reiff's suggestion (*Geschichte der Unendlichen Reihen*), to call the theorem the Euler-Maclaurin Summation Formula seems well justified.

Going still further back in time, the idea behind the trapezoidal rule (TR) (i.e., including the first term only in the RHS of (1)) has been traced back to around 50 BC [21]. A general rule for obtaining further correction terms (in the form of one-sided finite difference (FD)-type end corrections rather than increasing order derivatives) was given by James Gregory in 1670 [18], predating not only the EM formulas (by about 65 years), but also the first publications on calculus (by Leibniz in 1684 and Newton in 1687).

Some quadrature weights in the Gregory's formulas become negative for accuracies of orders 10 and above.[3] It was only recently noted that this onset of negative weights can be significantly delayed [15, 17]. The present study focuses on FD-type end corrections that are aligned with the line of integration, but are not (as with the Gregory formulas) confined to the interior if the interval. If

[2] For alternating sums, EM-like options include $\sum_{k=n}^{\infty}(-1)^k f(k) \approx \frac{(-1)^n}{2}\{f(n) - \frac{1}{2}f'(n) + \frac{1}{24}f'''(n) - \frac{1}{240}f^{(5)}(n) + \frac{17}{40370}f^{(7)}(n) - + \ldots\}$ (in which there is no integral term present).

[3] The same is the case for Newton-Cotes quadrature formulas.

an analytic function is to be integrated along a grid line in the complex plane, additional FD-type end correction opportunities arise [13, 14].

In this paper we describe some ways to re-formulate the EM formulas, such that infinite sums $\sum_{k=0}^{\infty} f(k)$ can be very accurately evaluated when only the anti-derivative

$$F(x) = -\int_{x}^{\infty} f(t)dt \tag{3}$$

(satisfying $F'(x) = f(x)$), or both $F(x)$ and $f(x)$ are conveniently available (i.e. without any need for analytic differentiations of $f(x)$). Either (1) or (2) can serve as the starting point for this task. To be specific, we focus here on the latter choice.

We note in Section 2.1 that truncating (2) to give accuracy $O(h^{2m})$, then replacing each derivative of $f(x)$ up through $f^{(2m-1)}(x_0)$ with regular centered FD approximations of $F(x)$ at $2m-1$ points,[4] spaced for example either h or $h/2$ apart, also becomes accurate to $O(h^{2m})$. Since the goal is to approximate a unit-spaced sum, we use $h = 1$ in the EM2 formula (2). For the FD approximations, we find that $h = 1/2$ provides an excellent trade-off between accuracy and sizes of coefficients.[5] The remaining parts of Section 2 give two additional approaches for creating the same weight set for $F(x)$ values, and also a simple error estimate. In Section 3, we consider Hermite-type FD (HFD) approximations, replacing some $F(x)$ evaluations with equally many $f(x)$ evaluations. Numerical tests in Section 4 show that the resulting accuracy now becomes nearly identical to having used analytical derivatives in (2) (in case such would have been available).

It is observed in Appendix A that the literature contains a large number of different derivations of the Euler-Maclaurin formulas, and Appendix B gives some general background on FD/HFD approximations.

2 FD approximations in the EM2 formula, using F-values only

From this point on, we set $h = 1$ in (2), and make it our task to approximate $\sum_{k=0}^{\infty} f(k + \frac{1}{2})$.[6]

In the following we let h instead stand for the FD step we use when approximating the derivatives that appear in the EM formulas.

2.1 Explicit FD approximations of even order derivatives

In terms of $F(x)$ (the anti-derivative of $f(x)$, as defined in (3)), equation (2) can be written as

$$\begin{aligned}\sum_{k=0}^{\infty} f(k+\frac{1}{2}) \approx -F(0) + \frac{1}{24}F^{(2)}(0) - \frac{7}{5760}F^{(4)}(0) + \frac{31}{967680}F^{(6)}(0) - \\ - \frac{127}{154828800}F^{(8)}(0) + \frac{73}{3503554560}F^{(10)}(0) - + \dots\end{aligned} \tag{4}$$

[4] These FD approximations are not the narrowest possible for the derivative in question, but of of optimal accuracy for the fixed stencil width $2m - 1$.

[5] Additionally, this choice of $h = 1/2$ leads to formulas that match those in [22], there arrived at from an entirely different perspective (not related to either EM formulas or FD approximations).

[6] When approximating an infinite sum $\sum_{k=0}^{\infty} f(k)$, it is a good strategy to first evaluate a number of leading terms $\sum_{k=0}^{N-1} f(k)$ before applying an asymptotic expansion to the remaining sum $\sum_{k=N}^{\infty} f(k)$. Re-defining $f(x)$ by a translation in x of size $N - \frac{1}{2}$ changes this latter sum to $\sum_{k=0}^{\infty} f(k + \frac{1}{2})$ and makes $x_0 = 0$.

If we decide for example to approximate the RHS of (4) by 5 values of $F(x)$, spaced $h = \frac{1}{2}$ apart, and centered around $x = 0$, the most accurate possibility (cf. Table 4, in Appendix B) would be to use

$$F^{(2)}(0) \approx 2^2 \left(-\frac{1}{12}F(-1) + \frac{4}{3}F(-\frac{1}{2}) - \frac{5}{2}F(0) + \frac{4}{3}F(\frac{1}{2}) - \frac{1}{12}F(1) \right),$$

and

$$F^{(4)}(0) \approx 2^4 \left(1F(-1) - 4F(-\frac{1}{2}) + 6F(0) - 4F(\frac{1}{2}) + 1F(1) \right).$$

With only 5 points, it is impossible to approximate higher than the 4^{th} derivative, so further terms in (4) need to be omitted.[7]

With the two FD formulas above, the weights we should apply to $\{F(-1),\ F(-\frac{1}{2}),\ F(0),\ F(\frac{1}{2}),\ F(1)\}$ in order to approximate the RHS of (4) become

$$\begin{array}{rrrrrrl}
-1\{ & 0, & 0, & 1, & 0, & 0, & \} \\
+\frac{1}{24}2^2\{ & -\frac{1}{12}, & \frac{4}{3}, & -\frac{5}{2}, & \frac{4}{3}, & -\frac{1}{12}, & \} \\
-\frac{7}{5760}2^4\{ & 1, & -4, & 6, & -4, & 1, & \} = \\
=\{ & -\frac{1}{30}, & \frac{3}{10}, & -\frac{23}{15}, & \frac{3}{10}, & -\frac{1}{30}, & \}
\end{array},$$

resulting in

$$\sum_{k=0}^{\infty} f(k + \frac{1}{2}) \approx -\frac{1}{30}F(-1) + \frac{3}{10}F(-\frac{1}{2}) - \frac{23}{15}F(0) + \frac{3}{10}F(\frac{1}{2}) - \frac{1}{30}F(1)\,. \tag{5}$$

We describe this as the $\mu = 3$ approximation, since it uses 3 terms in the RHS of (4). With this approach, one can readily generate the Table 1, which shows the corresponding results based on $\mu = 1, 2, \ldots, 6$ terms in (4). The last line ($\mu = 6$) utilizes all the terms written out explicitly in (4). EM formulas used to approximate sums always require $F(x)$ to be numerically available. When applying the approximations shown in Table 1, no function values or derivatives of $f(x)$ are used.

In the next two sections, we see how exactly this same sequence of increasing order approximations (as shown in Table 1) can be generated in additional ways.

2.2 Explicit FD approximation of the first derivative

Aiming again to arrive at (5), we can note that the order 6 approximation to the first derivative, as given in Table 4 (Appendix B) for $h = \frac{1}{2}$ becomes

$$f(k) \approx 2\left\{-\tfrac{1}{60}F(k-\tfrac{3}{2}) + \tfrac{3}{20}F(k-1) - \tfrac{3}{4}F(k-\tfrac{1}{2}) + 0F(k) + \tfrac{3}{4}F(k+\tfrac{1}{2}) - \tfrac{3}{20}F(k+1) + \tfrac{1}{60}F(k+\tfrac{3}{2})\right\}.$$

When summing this relation for $k = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$, the LHS becomes $\sum_{k=0}^{\infty} f(k + \frac{1}{2})$, and the RHS becomes a telescoping sum, with coefficients adding up as follows (at locations $-1, -\frac{1}{2}, 0, \frac{1}{2}, \ldots$):

[7] All FD and HFD formulas referred to in this study have the uniquely determined coefficients that make them exact for polynomials of as high degree as possible.

μ	$-\frac{5}{2}$	-2	$-\frac{3}{2}$	-1	$-\frac{1}{2}$	0	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$
	Weights for $F(x)$ at x-locations										
1						-1					
2					$\frac{1}{6}$	$-\frac{4}{3}$	$\frac{1}{6}$				
3				$-\frac{1}{30}$	$\frac{3}{10}$	$-\frac{23}{15}$	$\frac{3}{10}$	$-\frac{1}{30}$			
4			$\frac{1}{140}$	$-\frac{8}{105}$	$\frac{57}{140}$	$-\frac{176}{105}$	$\frac{57}{140}$	$-\frac{8}{105}$	$\frac{1}{140}$		
5		$-\frac{1}{630}$	$\frac{5}{252}$	$-\frac{38}{315}$	$\frac{125}{252}$	$-\frac{563}{315}$	$\frac{125}{252}$	$-\frac{38}{315}$	$\frac{5}{252}$	$-\frac{1}{630}$	
6	$\frac{1}{2772}$	$-\frac{2}{385}$	$\frac{25}{693}$	$-\frac{568}{3465}$	$\frac{1585}{2772}$	$-\frac{6508}{3465}$	$\frac{1585}{2772}$	$-\frac{568}{3465}$	$\frac{25}{693}$	$-\frac{2}{385}$	$\frac{1}{2772}$

Table 1: Weights for $F(x)$ at different x-locations when approximating $\sum_{k=0}^{\infty} f(k+\frac{1}{2})$.

$$
\begin{array}{rcccccccccccc}
2\{ & -\frac{1}{60}, & \frac{3}{20}, & -\frac{3}{4}, & 0, & \frac{3}{4}, & -\frac{3}{20} & \frac{1}{60}, & 0, & 0, & 0, & 0, & \ldots\} \\
+\,2\{ & & & -\frac{1}{60}, & \frac{3}{20}, & -\frac{3}{4}, & 0, & \frac{3}{4}, & -\frac{3}{20} & \frac{1}{60}, & 0, & 0, & \ldots\} \\
+\,2\{ & & & & & -\frac{1}{60}, & \frac{3}{20}, & -\frac{3}{4}, & 0, & \frac{3}{4}, & -\frac{3}{20} & \frac{1}{60}, & \ldots\} \\
+\,2\{ & & & & & & & -\frac{1}{60}, & \frac{3}{20}, & -\frac{3}{4}, & 0, & \frac{3}{4}, & \ldots\} \\
+\,2\{ & & & & & & & & & -\frac{1}{60}, & \frac{3}{20}, & -\frac{3}{4}, & \ldots\} \\
+\,2\{ & & & & & & & & & & & -\frac{1}{60}, & \ldots\} + \ldots = \\
=\{ & -\frac{1}{30}, & \frac{3}{10}, & -\frac{23}{15}, & \frac{3}{10}, & -\frac{1}{30}, & 0, & 0, & 0, & 0, & 0, & 0, & \ldots\}.
\end{array}
$$

The expression in the bottom line exactly reproduces (5), with corresponding agreements (with Table 1) when extended to arbitrary orders of accuracy. A closed form expression for the 1^{st} derivative approximations (shown in Table 4 for orders $p = 2, 4, 6, 8$) follow from Lagrange's interpolation formula. For order p (even),

$$w_0^{(p)} = 0 \quad \text{and} \quad w_j^{(p)} = \frac{(-1)^{j+1}(p/2)!^2}{j(p/2+j)!(p/2-j)!}, \qquad j = \pm 1, \pm 2, \ldots, \pm p/2.$$

This approach, based on a single FD approximation of the first derivative, requires no knowledge of the expansion (2) (and, in particular, that this expansion has coefficients that involve Bernoulli numbers; cf., the derivations in Appendix A).

2.3 Generating function approach

To arrive at the weights in Table 1 in yet another way, it is convenient in our present case $h = \frac{1}{2}$ to define a centered difference operator $\triangle$ by

$$\triangle\, F(k) = F(k + \frac{1}{4}) - F(k - \frac{1}{4}).$$

Then

$$\triangle^2\, F(0) = \triangle\, (\triangle\, F(0)) = F(-\frac{1}{2}) - 2F(0) + F(\frac{1}{2}),$$

$$\triangle^4\, F(0) = F(-1) - 4F(-\frac{1}{2}) + 6F(0) - 4F(\frac{1}{2}) + F(1),$$

etc. We seek an expansion of the form

$$\sum_{k=0}^{\infty} f(k+\frac{1}{2}) \approx \sum_{n=0}^{\infty} a_n \, \triangle^{2n} \, F(0). \tag{6}$$

Choosing as 'test function' for example $F(x) = e^{zx}$ gives $f(x) = ze^{zx}$, $\sum_{k=0}^{\infty} f(k+\frac{1}{2}) = \frac{ze^{z/2}}{1-e^z}$, and $\triangle^2 \, F(0) = 4\left(\sinh\frac{z}{4}\right)^2$, $\triangle^4 \, F(0) = 4^2\left(\sinh\frac{z}{4}\right)^4$, etc. Next, substituting $4\left(\sinh\frac{z}{4}\right)^2 = t$, i.e. $z = 4\,\mathrm{arcsinh}\frac{\sqrt{t}}{2}$ gives, after a few simplifications[8]

$$\sum_{k=0}^{\infty} f(k+\frac{1}{2}) = \frac{ze^{z/2}}{1-e^z} = \frac{-4\mathrm{arcsinh}\frac{\sqrt{t}}{2}}{\sqrt{t}\sqrt{t+4}} = \sum_{n=0}^{\infty} \frac{(-1)^{n+1}(n!)^2}{(2n+1)!} t^n.$$

Since $\triangle^2 \, F(0) = t$, this should (in view of (6)) match $\sum_{n=0}^{\infty} a_n t^n$, from which we thus read off[9]

$$a_n = \frac{(-1)^{n+1}(n!)^2}{(2n+1)!}, \quad n = 0, 1, 2, \ldots \tag{7}$$

In the same $\mu = 3$ demonstration case as above, combining (6) and (7) gives the $F(x)$ weights

$$\begin{array}{rlllllll}
-\frac{(0!)^2}{1!} & \{ & 0, & 0, & 1, & 0, & 0 & \} \\
+\frac{(1!)^2}{3!} & \{ & 0, & 1, & -2, & 1, & 0 & \} \\
-\frac{(2!)^2}{5!} & \{ & 1, & -4, & 6, & -4, & 1 & \} = \\
= & \{ & -\frac{1}{30}, & \frac{3}{10}, & -\frac{23}{15}, & \frac{3}{10}, & -\frac{1}{30} & \} \quad .
\end{array}$$

Also this approach extends immediately to higher orders / wider stencils. For a given value of μ and at locations $x = k/2$, $k = 0, \pm 1, \pm 2, \ldots, \pm(\mu-1)$, it gives the following closed form expression for the weights in Table 1:

$$w_{\mu,k} = (-1)^{k+1} \sum_{n=|k|}^{\mu-1} \frac{(n!)^2}{(2n+1)(n+k)!(n-k)!}. \tag{8}$$

From this follows that $|w_{\mu,k}| \leq \sum_{n=0}^{\mu-1} \frac{1}{2n+1}$, implying that there is no risk of dangerous numerical cancellations even if using large numbers μ of EM terms.

2.4 Error estimates

The estimates below aim to be practical to use, rather than rigorous.[10] If we include μ terms in the RHS of (4), the error becomes roughly the size of the first omitted term, i.e.

$$\mathrm{EM2}_{\mathrm{Error}} \approx \frac{B_{2\mu}}{(2\mu)!} F^{(2\mu)}(0) \approx \frac{2}{(2\pi)^{2\mu}} F^{(2\mu)}(0). \tag{9}$$

[8]The last equality follows from noting that $y(x) = \frac{\mathrm{arcsinh}\frac{x}{2}}{\sqrt{4+x^2}}$ satisfies the ODE $(4+x^2)y'(x) + xy - 1 = 0$, $y(0) = 0$; equating coefficients gives $y(x) = \frac{1}{4}\sum_{n=0}^{\infty} \frac{(-1)^n (n!)^2}{(2n+1)!} x^{2n+1}$.

[9]Equations (6), (7) can be expressed as the identity $\sum_{n=0}^{\infty} \frac{B_{2n}}{(2n)!}(1-2^{1-2n})F^{(2n)}(0) = \sum_{n=0}^{\infty} \frac{(-1)^{n+1}(n!)^2}{(2n+1)!} \, \triangle^{2n} \, F(0)$ for all polynomials $F(x)$.

[10]If $F(x)$ is 'totally monotone', more strict arguments can be based on 'semi-convergence', cf., [19], pages 328-329. With "≈" in (9), (10), we refer to magnitude (and not sign).

The three approaches in Sections 2.1-2.3 all led to the identical approximations, with weights as shown in Table 1. Of these approaches, the one in Section 2.3 leads most easily to an error estimate if we again approximate the error with the first omitted term:

$$\text{FD}_{\text{Error}} \approx \frac{(\mu!)^2 2^{-2\mu}}{(2\mu+1)!} F^{(2\mu)}(0) \approx \frac{1}{4^{2\mu}} \frac{1}{2} \sqrt{\frac{\pi}{\mu}} F^{(2\mu)}(0). \tag{10}$$

This FD version approximates (4) up through its first μ terms. At whatever level EM2 has been truncated, comparing (10) with (9) shows that (10) has lost approximately $2\mu \log_{10}\left(\frac{\pi}{2}\right) \approx 0.39\mu$ decimal digits (in excellent agreement with what we will later see in Figure 2).

2.5 Further opportunities for improving the accuracy of the FD approximations

The following possibilities can be considered:

1. One can use a smaller step h (than $h = \frac{1}{2}$) when approximating the derivatives in (4). The approaches in Sections 2.1 and 2.3 (but not the one in Section 2.2, nor the one in [22]) generalize immediately to arbitrary FD step size h. However, reducing h (below $h = \frac{1}{2}$) will make the weights grow rapidly in magnitude, introducing dangers of numerical cancellations.
2. FD approximations for increasingly high order derivatives tend to be ill-conditioned if functional data is available only along the real axis. However, using values of an analytic function at locations in the complex plane surrounding the point of interest, makes the task numerically stable [6, 10]). This was utilized for EM-type end corrections in [13, 14]. In this study we want to rely on real-valued calculations only.
3. We can replace some $F(x)$ evaluations with equally many $f(x)$ evaluations, borrowing the key idea from Hermite-type finite differences. This is followed up on next.

3 Hermite-type FD (HFD) approximations using both F- and f-values

Recalling that $F'(x) = f(x)$, the terms after the first one in the RHS of (4) can just as well be written as $\frac{1}{24} f^{(1)}(0) - \frac{7}{5760} f^{(3)}(0) + \frac{31}{96780} f^{(5)}(0) - + \ldots$, which then can be approximated with an anti-symmetric FD operator applied to equi-spaced $f(x)$-values. Either of these two versions, i.e., use F-values only (as previously), or use just one F-value and then only f-values, can be viewed as two opposite extremes. We note in each of the Sections 3.1-3.3 a different option for generating Hermite-type weight sets, using half F- and half f-values. The last of the three approaches is much preferable with regard to numerical stability, computational speed, and ease of use. It is based on explicit recursions (instead of requiring solutions to often ill-conditioned linear systems).

3.1 Direct enforcement of accuracy

Using again as an example the first three terms in the RHS of (4)), the task now becomes to make

$$\left\{ -F(0) + \frac{1}{24} F^{(2)}(0) - \frac{7}{5760} F^{(4)}(0) \right\} = \{a_1 F(-h) + a_0 F(0) + a_1 F(h)\} + \{-b_1 f(-h) + b_1 f(h)\} \tag{11}$$

valid for as high degree polynomials $F(x)$ as possible. This equation is exact whenever $F(x)$ is an odd function (as both sides then evaluate to zero). Requiring it to hold also for $F(x) = 1, x^2, x^4$

gives 3 linear equations in the 3 unknowns $\{a_0, a_1, b_1\}$. Solving for these then makes (11) exact for all polynomials up through degree 5.[11] Equation (11) generalizes in an obvious way to higher order approximations.

3.2 Cauchy integral method

An analytically elegant approach to obtain a linear system for $\{a_0, a_1, b_1\}$ from (11) (leading to the same result) was introduced, in a different context, in [7]; see also [8]. Recalling Cauchy's integral formula

$$\frac{F^{(n)}(x)}{n!} = \frac{1}{2\pi i} \oint_C \frac{F(z)}{(z-x)^{n+1}} dz \ ,$$

we can alternatively express (11) as requiring

$$\frac{1}{2\pi i} \oint_C F(z) \left\{ \left(-\frac{1}{z} + \frac{1}{24}\frac{2!}{z^3} - \frac{7}{5760}\frac{4!}{z^5} \right) - \left(\frac{a_1}{z+h} + \frac{a_0}{z} + \frac{a_1}{z-h} \right) - \left(-\frac{b_1}{(z+h)^2} + \frac{b_1}{(z-h)^2} \right) \right\} dz = 0 \qquad (12)$$

for as high degree polynomials $F(z)$ as possible. Putting the rational terms in the integrand on a common denominator gives an expression of the form $\frac{p_8(z)}{z^5(z+h)^2(z-h)^2}$, where $p_8(z)$ is an even polynomial of degree 8. Requiring this polynomial's coefficients for z^8, z^6, z^4 to be zero gives again a linear system for $\{a_0, a_1, b_1\}$. The degree of $p_8(z)$ has then dropped to 2, implying (by choosing the contour C large) that (12) (and thereby also (11)) will evaluate to zero whenever $F(z)$ is a polynomial up through degree 5.

3.3 Hermite-type FD formulas

The function *weights* mentioned in Appendix B (with MATLAB code in Appendix B of [12]) produces not only all the FD formulas that have been referred to above, but also Hermite-type FD formulas for $f^{(k)}(z)$, $k = 0, 1, \ldots, m$ based on both $f(x)$ and $f'(x)$ values at a node set $x = x_1, x_2, \ldots, x_n$ (using only computationally fast and stable explicit recursions). Changing notation $f(x) \to F(x)$ and $f'(x) \to f(x)$ (to agree with conventions elsewhere in this paper), a call to *weights* with, for ex. $z = 0$, $x = [-2, -1, 0, 1, 2]$, $m = 5$ produces in the output variable c the 5-node wide formulas in Table 4 and in variables d and e Hermite 5-node wide Hermite sets of twice the accuracy order. Calling *weights* with $z = 0$, $x = [-\frac{1}{2}, 0, \frac{1}{2}]$, $m = 5$ produces similarly in d and e the formulas shown in Table 2. The lines for $F(0)$, $F^{(2)}(0)$, $F^{(4)}(0)$ in this Table 2, combined together according to (4), produce the two $\mu = 3$ lines in Table 3. Any other line in this Table 3 (as well as any further pair of lines) follow likewise from a single call to this MATLAB function *weights*.[12]

4 Numerical tests

We consider next two numerical examples:

[11] As in the case of (5), the approximation (11) is based on $\mu = 3$ non-trivial coefficients and its application requires a total of $2\mu - 1 = 5$ function evaluations (here 3 for F and 2 for f).

[12] While all the weights in Table 3 are rational numbers, it remains unclear if there is any practical closed form expression available for them (corresponding to (8) in the case of FD approximations). Although the numerators and denominators in Table 3 grow quite rapidly with μ, this growth is well less than that of the EM2 expansion they are based on. For example, the $\mu = 11$ EM2 term has a coefficient that is a ratio between an 11 digit and a 27 digit integer, while no numerator or denominator in Table 3 has more than 10 digits.

	Weights at									
	$x =$	$-\frac{1}{2}$	0	$+\frac{1}{2}$		$x =$	$-\frac{1}{2}$	0	$+\frac{1}{2}$	
$F(0) \approx$	[	0	1	0	$]F$	$+$ [	0	0	0	$]f$
$F^{(1)}(0) \approx$	[	0	0	0	$]F$	$+$ [	0	1	0	$]f$
$F^{(2)}(0) \approx$	8 [	1	-2	1	$]F$	$+$ [	1	0	-1	$]f$
$F^{(3)}(0) \approx$	60 [	-1	0	1	$]F$	$+6$ [	-1	-8	-1	$]f$
$F^{(4)}(0) \approx$	192 [	-1	-2	-1	$]F$	$+48$ [	-1	0	1	$]f$
$F^{(5)}(0) \approx$	2880 [	1	0	-1	$]F$	$+480$ [	1	4	1	$]f$

Table 2: The weight set produced when the MATLAB function *weights* (described in Appendix B) is called with the parameters $z = 0,\ x = [-\frac{1}{2}, 0, \frac{1}{2}],\ m = 5$.

Number μ of EM2 terms included	Weight at x-coordinate					
	0	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$
	a-coefficients (applied to $F(x)$)					
1	-1					
3	$-\frac{32}{15}$	$\frac{17}{30}$				
5	$-\frac{446}{105}$	$\frac{2447}{1890}$	$\frac{311}{945}$			
7	$-\frac{137728}{15015}$	$\frac{116713}{60060}$	$\frac{151808}{75075}$	$\frac{1101}{9100}$		
9	$-\frac{17037278}{765765}$	$\frac{22542743}{15315300}$	$\frac{2279888}{294525}$	$\frac{147177473}{107207100}$	$\frac{1037501}{26801775}$	
11	$-\frac{873168704}{14549535}$	$-\frac{275237747}{58198140}$	$\frac{2564157952}{101846745}$	$\frac{6800077217}{814773960}$	$\frac{643343968}{916620705}$	$\frac{85167469}{7332965640}$
	b-coefficients (applied to $f(x)$)					
1	0					
3	0	$-\frac{1}{10}$				
5	0	$-\frac{67}{126}$	$-\frac{5}{126}$			
7	0	$-\frac{1601}{858}$	$-\frac{896}{2145}$	$-\frac{53}{4290}$		
9	0	$-\frac{144967}{24310}$	$-\frac{2184}{935}$	$-\frac{37537}{170170}$	$-\frac{303}{85085}$	
11	0	$-\frac{158733}{8398}$	$-\frac{306944}{29393}$	$-\frac{212837}{117572}$	$-\frac{25696}{264537}$	$-\frac{1049}{1058148}$

Table 3: a- and b-coefficients when (11) is extended to increasingly many terms in its left bracket, and with $h = \frac{1}{2}$. The a-coefficients should be extended symmetrically and the b-coefficients anti-symmetrically across $x = 0$.

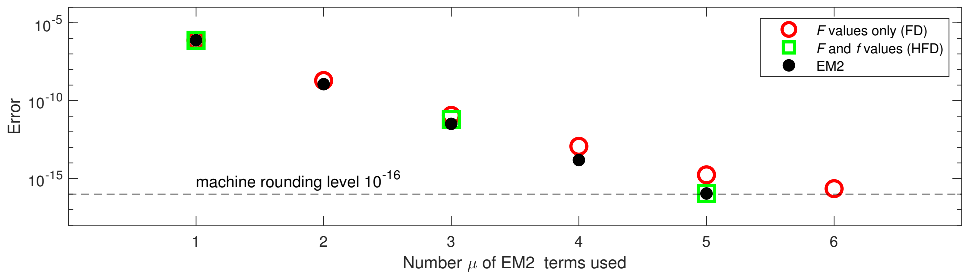

Figure 1: Errors in Example 1 when using the two different FD approaches.

Example 1: Approximate $\sum_{k=1}^{\infty} f(k) \approx 0.25903856926239039237$ where

$$f(x) = \frac{x \,\text{erfinv}(\arctan \frac{1}{\sqrt{1+x^2}})}{(x^2+2)\sqrt{1+x^2}},$$
$$F(x) = \frac{e^{-(\text{erfinv}(\arctan \frac{1}{\sqrt{1+x^2}}))^2} - 1}{\sqrt{\pi}}.$$

The sum converges, since $f(x) = O(1/x^3)$ for $x \to \infty$.[13] We (quite arbitrarily) choose to sum $\sum_{k=1}^{19} f(k)$ explicitly, and then apply EM2, the FD, and the HFD schemes to $\sum_{k=20}^{\infty} f(k)$. Using in turn all the $\mu = 1, 2, \ldots, 6$ rows of Table 1 and (separately) the top three rows in each part of Table 3 (for $\mu = 1, 3, 5$) give the errors in the final sum as shown by open red circles and green squares, respectively, in Figure 1. These calculations were done in regular double precision arithmetic, with roughly 16 decimal digits of precision. Applying EM2 with analytic derivatives is barely possible since, already for $\mu = 5$, the analytic form for $\frac{d^7}{dx^7} f(x)$ is a multi-page-sized expression. The EM2 results are shown as filled black circles. The loss in accuracy for the (computationally vastly faster) FD and HFD approximations is hardly noticeable.

Example 2: Approximate the Euler-Mascheroni constant

$$\gamma = \lim_{n\to\infty} \left(\sum_{k=1}^{n} \frac{1}{k} - \log n \right) = 1 + \sum_{k=2}^{\infty} \left(\frac{1}{k} + \log(k-1) - \log(k) \right) \approx 0.57721566490153286061 \quad (13)$$

by directly summing $\sum_{k=2}^{N-1}$ and then applying EM2 and its FD and HFD approximations to $\sum_{k=N}^{\infty}$.

In this example,

$$f(x) = \frac{1}{x} + \log(1 - \frac{1}{x}),$$
$$F(x) = 2(x-1)\text{arccoth}(2x-1) - 1.$$

The example is chosen because (atypically) vast numbers of analytic derivatives can be taken very conveniently. Figure 2 shows how the resulting accuracy varies with μ (the number of EM2 terms included).[14] The bottom curve (filled black circles) in each of the three different cases (of $N = 10,\ 60,\ 300$) shows the errors when applying EM2 exactly. Using μ EM2 terms directly requires the evaluations of f-derivatives up through order $2\mu - 1$.

[13] This function $f(x)$ was previously considered as Example 6.2 in [22].

[14] Extended precision arithmetic was implemented using the Advanpix package [2].

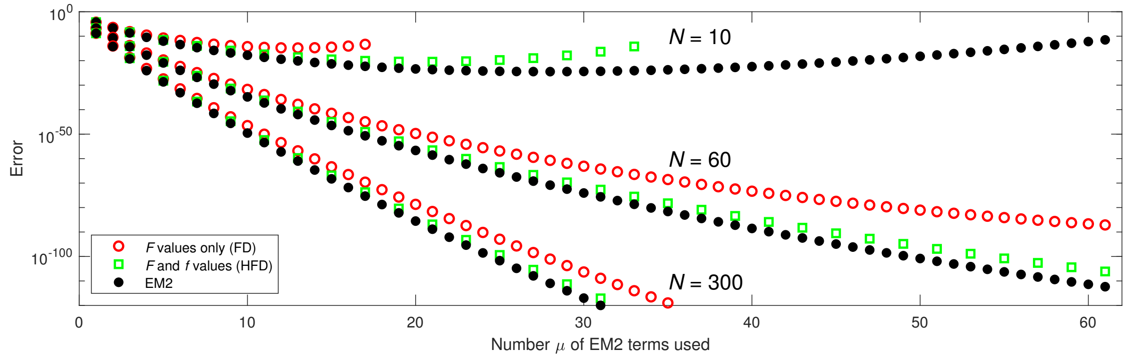

Figure 2: Errors in the numerical test problem in cases of $N = 10,\ 60,\ 300$. In each of these three cases, the bottom curve shows the error when successively increasing number μ of EM2 terms have been implemented exactly (requiring analytic derivatives of $f(x)$ up through order $2\mu - 1$). For each of these cases, the two curves above it illustrate the achieved accuracy when these same EM2 terms instead have been implemented by means of $(2\mu - 1)$ $F(x)$ evaluations (red circles), and by μ $F(x)$ evaluations together with $(\mu - 1)$ $f(x)$ evaluations, respectively (green squares).

The FD approach (replacing μ EM2 terms with $(2\mu-1)$ F-evaluations; open red circles) is seen to loose decimal digits in excellent agreement with the estimate $2\mu \log_{10}\left(\frac{\pi}{2}\right) \approx 0.39\mu$ given in Section 2.4. The HFD approach (using μ $F(x)$-evaluations together with $(\mu - 1)$ f-evaluations; open green squares) is seen to result in near-optimal accuracy (given the EM2 expansion it is based on).

The most cost-effective choice for the two parameters N and μ will depend on the desired level of accuracy. If we wish to reach here an error level around 10^{-50}, then $N = 10$ is seen to be out of question. Given that the cost for either FD or HFD is $2\mu - 1$ function evaluations, choosing $N = 60$ and μ around 30 will be cheaper than any calculation starting with $N \gtrsim 120$ initial terms to sum.

Just as with the EM formulas (and also for most other asymptotic expansions), monitoring the change in result when increasing the number of terms (here μ) provides easy-to-obtain (practical, but non-rigorous) error estimates.

Comment on numerical stability: Hermite-type FD formulas can be very attractive for solving PDEs, then typically used to approximate only low order derivatives [1]. A minor issue arises in contexts (such as the present one) that involve very high order derivatives, since the weights then may then grow in size. While there were no growth issues for increasing μ in Table 1 (cf., equation (8)), the largest entry in Table 3 ($\mu = 11$) has magnitude $\frac{873168704}{14549535} \approx 60$. For $\mu = 31$ and $\mu = 61$, the corresponding sizes become approximately 10^7 and 10^{15}, respectively, meaning that 7 and 15 extra digits of extended precision are then needed to off-set possible numerical cancellations. However, once extended precision has been invoked (coming at a significantly increased cost relative to hardware implemented double precision), the extra cost in such relatively minor further increases in precision is insignificant.

5 Conclusions

The two Euler-Maclaurin (EM) formulas have been known for centuries, derived independently by Euler and Maclaurin around 1735.[15] Approximating derivatives with finite differences can be

[15] Focusing on accelerating the convergence of infinite sums, and on approximating integrals, respectively.

traced back even further. The present novelty is that the high order derivatives these EM formulas contain can be safely replaced by either 'regular' centered FD or by (also centered) Hermite-based FD approximations. The present results, focusing on EM2, all have closely related counterparts if instead using the EM1 approximation.

6 Appendix A: Some derivations of the Euler-Maclaurin formulas

The original derivations by Euler and Maclaurin are described (with additional historical notes) in [9, 20]. A remainder term was introduced by Poisson in 1823. Numerous derivations can be found in contemporary text books, often utilizing Bernoulli polynomials and integrations by parts (e.g., [3, 4, 5, 23]). We limit the discussion here to sketching out three additional approaches.

6.1 Generating function approach to obtain expansion coefficients

The coefficients in (1), (2) follow from a *generating function* approach. For notational simplicity, we shift the function $f(x)$ so that $x_0 = 0$. Consider then functions $f(x) = e^{z\,x}$ with z in the complex left half-plane. Substituting this into (1) and (2) gives

$$\int_0^\infty f(x)dx - h\sum_{k=0}^{\infty} f(kh) = \frac{h}{e^{hz}-1} - \frac{1}{z} = \sum_{k=1}^{\infty} \frac{B_k h^k}{k!} z^{k-1} = \tag{14}$$
$$-\frac{h}{2} + \frac{h^2}{12}z - \frac{h^4}{720}z^3 + \frac{h^6}{30240}z^5 - \frac{h^8}{1209600}z^7 + - \ldots$$

and

$$\int_0^\infty f(x)dx - h\sum_{k=0}^{\infty} f((k+\frac{1}{2})h) = h\frac{e^{hz/2}h}{e^{hz}-1} - \frac{1}{z} = -\sum_{k=1}^{\infty} \frac{B_k h^k}{k!}(1-2^{1-k}) z^{k-1} = \tag{15}$$
$$-\frac{h^2}{24}z + \frac{7\,h^4}{5760}z^3 - \frac{31\,h^6}{967680}z^5 + \frac{127\,h^8}{154828800}z^7 + - \ldots\ ,$$

where we recognize all the coefficients from (1) and (2). Here, B_k is known as the k^{th} Bernoulli number (with $B_k = 0$ for $k = 3, 5, 7, \ldots$). Since 2^{1-k} becomes small compared to 1 as k increases, the sizes of the coefficients are comparable in (14) and (15). We conclude by noting that $f(x) = e^{z\,x}$ implies that $f^{(k)}(0) = z^k$.

The two expansions are closely related; EM2 can be seen as an immediate consequence of EM1 by means of the trivial identity

$$[\frac{1}{2}f(0) + f(\frac{1}{2}h) + f(1h) + f(\frac{3}{2}h) + f(2h) + \ldots] - [\frac{1}{2}f(0) + f(1h) + f(2h) + \ldots] =$$
$$= [f(\frac{1}{2}h) + f(\frac{3}{2}h) + f(\frac{5}{2}h) + \ldots]$$

.

6.2 Sketch of derivation via telescoping series

The definition of Bernoulli numbers appeared above in (14):

$$\frac{z}{e^z-1}=\sum_{n=0}^{\infty}\frac{B_n}{n!}z^n. \tag{16}$$

We next multiply (16) by the denominator in its LHS and equate coefficients for z. The result can be expressed in matrix form as

$$\begin{bmatrix} \frac{1}{1!} & \frac{1}{2!} & \ddots & \frac{1}{n!} \\ & \frac{1}{1!} & \frac{1}{2!} & \ddots \\ & & \ddots & \ddots \\ & & & \frac{1}{1!} \end{bmatrix}^{-1} = \begin{bmatrix} \frac{B_0}{0!} & \frac{B_1}{1!} & \ddots & \frac{B_{n-1}}{(n-1)!} \\ & \frac{B_0}{0!} & \frac{B_1}{1!} & \ddots \\ & & \ddots & \ddots \\ & & & \frac{B_0}{0!} \end{bmatrix}, \tag{17}$$

$n=1,2,3,\ldots$ (with both matrices upper triangular and constant along each diagonal).

From the Taylor expansion

$$f(x)=f(k)+\frac{1}{1!}(x-k)f'(k)+\frac{1}{2!}(x-k)^2f''(k)+\ldots$$

follows (focusing for notational simplicity on the case of $h=1$) that

$$\begin{bmatrix} \int_k^{k+1} f(x)dx \\ f(k+1)-f(k) \\ f'(k+1)-f'(k) \\ \vdots \\ \end{bmatrix} = \begin{bmatrix} \frac{1}{1!} & \frac{1}{2!} & \frac{1}{3!} & \ddots \\ & \frac{1}{1!} & \frac{1}{2!} & \ddots \\ & & \frac{1}{1!} & \ddots \\ & & & \ddots \end{bmatrix} \begin{bmatrix} f(k) \\ f'(k) \\ f''(k) \\ \vdots \\ \end{bmatrix}.$$

Adding these relations for $k=0,1,2,\ldots$ gives telescoping sums in the LHS. Then applying (17) gives

$$\begin{bmatrix} \frac{B_0}{0!} & \frac{B_1}{1!} & \frac{B_2}{2!} & \ddots \\ & \frac{B_0}{0!} & \frac{B_1}{1!} & \ddots \\ & & \frac{B_0}{0!} & \ddots \\ & & & \ddots \end{bmatrix} \begin{bmatrix} \int_0^{\infty} f(x)dx \\ -f(0) \\ -f'(0) \\ \vdots \\ \end{bmatrix} = \begin{bmatrix} \sum_{k=0}^{\infty} f(k) \\ \sum_{k=0}^{\infty} f'(k) \\ \sum_{k=0}^{\infty} f''(k) \\ \vdots \\ \end{bmatrix}.$$

EM1 can now be read off from the top row of this relation.

6.3 Sketch of derivation via contour integration

If one assumes $f(z)$ is analytic and goes to zero in the right half-plane, contour integration gives in the EM2 case[16]

$$\int_0^{\infty} f(x)dx - h\sum_{k=0}^{\infty} f((k+\tfrac{1}{2})h) = i\int_0^{\infty}\frac{f(iy)-f(-iy)}{1+e^{2\pi y/h}}dy\ . \tag{18}$$

[16]Following G. Plana (1820) and N.H. Abel (1823). A contemporary description (in the EM1 case) can be found in Section 12.5.2.2 of [16].

The integral in the RHS often converges very rapidly (due to the exponential in the denominator). Taylor expanding $f(iy)$ around the origin makes (18) asymptotic rather than exact. Each resulting RHS term can be evaluated exactly, providing yet another way to arrive at EM2.

7 Appendix B: Fast generation of FD and HFD approximations

FD approximations to derivatives on equi-spaced grids were used to approximate ODEs already in the 19^{th} century, and have been applied to PDEs since the early 20^{th} century. Many tables and also closed form expressions for weights are available. The present Table 4 contains the same information as Table 3.1-1 in [11]. Earlier in this paper, Table 2 gave an illustration of some Hermite-type FD weights. For every one of the FD-based methods that have been discussed above (of 'regular' or of Hermite type), one single call to the short MATLAB function *weights* (described in [12], with the compete code listed in its Appendix A) computes all the weights needed. Either MATLAB's vpa (symbolic toolbox, variable precision arithmetic) or the extended precision package by Advanpix [2] provide arbitrary high arithmetic precision. The former also offers the choice of using exact rational arithmetic (in place of floating point arithmetic).

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Order of accuracy	-4	-3	-2	-1	0	1	2	3	4
0th derivative									
∞					1				
1st derivative									
2				$-\frac{1}{2}$	0	$\frac{1}{2}$			
4			$\frac{1}{12}$	$-\frac{2}{3}$	0	$\frac{2}{3}$	$-\frac{1}{12}$		
6		$-\frac{1}{60}$	$\frac{3}{20}$	$-\frac{3}{4}$	0	$\frac{3}{4}$	$-\frac{3}{20}$	$\frac{1}{60}$	
8	$\frac{1}{280}$	$-\frac{4}{105}$	$\frac{1}{5}$	$-\frac{4}{5}$	0	$\frac{4}{5}$	$-\frac{1}{5}$	$\frac{4}{105}$	$-\frac{1}{280}$
2nd derivative									
2				1	-2	1			
4			$-\frac{1}{12}$	$\frac{4}{3}$	$-\frac{5}{2}$	$\frac{4}{3}$	$-\frac{1}{12}$		
6		$\frac{1}{90}$	$-\frac{3}{20}$	$\frac{3}{2}$	$-\frac{49}{18}$	$\frac{3}{2}$	$-\frac{3}{20}$	$\frac{1}{90}$	
8	$-\frac{1}{560}$	$\frac{8}{315}$	$-\frac{1}{5}$	$\frac{8}{5}$	$-\frac{205}{72}$	$\frac{8}{5}$	$-\frac{1}{5}$	$\frac{8}{315}$	$-\frac{1}{560}$
3rd derivative									
2			$-\frac{1}{2}$	1	0	-1	$\frac{1}{2}$		
4		$\frac{1}{8}$	-1	$\frac{13}{8}$	0	$-\frac{13}{8}$	1	$-\frac{1}{8}$	
6	$-\frac{7}{240}$	$\frac{3}{10}$	$-\frac{169}{120}$	$\frac{61}{30}$	0	$-\frac{61}{30}$	$\frac{169}{120}$	$-\frac{3}{10}$	$\frac{7}{240}$
4th derivative									
2			1	-4	6	-4	1		
4		$-\frac{1}{6}$	2	$-\frac{13}{2}$	$\frac{28}{3}$	$-\frac{13}{2}$	2	$-\frac{1}{6}$	
6	$\frac{7}{240}$	$-\frac{2}{5}$	$\frac{169}{60}$	$-\frac{122}{15}$	$\frac{91}{8}$	$-\frac{122}{15}$	$\frac{169}{60}$	$-\frac{2}{5}$	$\frac{7}{240}$

(Column header spanning -4 to 4: Approximations at $x = 0$; x coordinates at nodes)

Table 4: Weights for some centered FD formulas on a unit-spaced grid. Applied to $F(x)$, they give approximations (at $x = 0$) to $F^{(k)}(x) = f^{(k-1)}(x)$. $k = 0, 1, \ldots, 4$. If the grid has spacing h, all first derivative weights need to be divided by h, all second derivative weights by h^2, etc.

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