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TRUNCATION ERROR FOR THE SIMPSON'S 1/3 RULE BASED ON TAYLOR SERIES EXPANSION

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Abstract. *This paper presents a deduction of the truncation error for the Simpson's 1/3 Rule as a series that can be used to code verification. Instead of using the classical approach of integration of interpolating polynomials, it uses the integration of the function expanded in Taylor Series. As result, the series is truncated after some terms. In this paper, it is deduced up to the third term. As well known, the Simpson's 1/3 Rule has asymptotic order four, and the deduction presented here allows to conclude that the true orders constitute the arithmetic progression: 4, 6, 8, … By using Repeated Richardson Extrapolation, the apparent orders of the truncation error are confirmed a posteriori by testing polynomials and exponential functions. In addition, the deduced equation is able to calculate the truncation error exactly for all tested functions that has a finite number of non-null derivatives.*

Keywords: *Simpson's 1/3 Rule, Repeated Richardson Extrapolation, Truncation Error Equation, Code Verification, Solution Verification*

1. INTRODUCTION

As the memory and processing speed of computers increase over time, the computational sciences develop as well as the complexity of the solved mathematical models (Oberkampf and Roy, 2010). As computer codes became complex and large, it becomes difficult to ensure that the code is error free (Knupp and Salari, 2002). Thus, a very important question arises: what is the confidence that a numerical solution correctly represents the solution of the mathematical model chosen to describe a specific phenomenon, equipment or physical process? This question is asked by a person responsible for writing the mathematical model in a computer code and solving it.

Knupp and Salari (2002) details a procedure that convincingly demonstrate through grid refinement that, for the problem of interest, the numerical solution produced by the code converges at the correct rate to the exact solution. The authors call this procedure Order Verification via the Manufactured Solution Procedure (OVMSP).

One step in the OVMSP is the determination of the theoretical order-of-accuracy. Ideally, the predicted and observed order-of-accuracy must agree. If not, one suspects the occurrence of a code mistake or error of implementation.

Some very important classes of problems deal with numerical integration, for example, neutron transport and radiative heat transfer. Furthermore, as the numerical integration is often used to compute post-processing variables (e.g. overall heat transfer rate, drag force over a solid surface), then the order-of-accuracy of those variables also need to be accounted for the verification of that part of the code (Knupp and Salari, 2002).

The present work uses Taylor Series Expansion to provide the asymptotic and following orders that appears when deducing the Simpson's 1/3 Rule with the Finite Difference Method. This procedure is similar to that presented in (Leonard, 1994, 1995) for the well-known Upwind Differencing Scheme (UDS), Central Differencing Scheme (CDS) and Quadratic Upwind Differencing Scheme (QUICK). The motivation behind this study is the possible use of the post-processing procedure called Repeated Richardson Extrapolation (RRE) in the OVMSP, as pointed out by Roache (2009).

The truncation error reported in this work is especially useful when approximations of different orders are mixed (Roache, 2009).

In the Finite Difference Method, the domain is subdivided in N elements, separated by $N+1$ grid points where the dependent variable F is available. For a uniform grid (i.e. all discrete elements have same length), as shown in Fig. 1, some internal points are represented: $j-1$, j and $j+1$, with respective positions x_{j-1}, x_j and x_{j+1}.

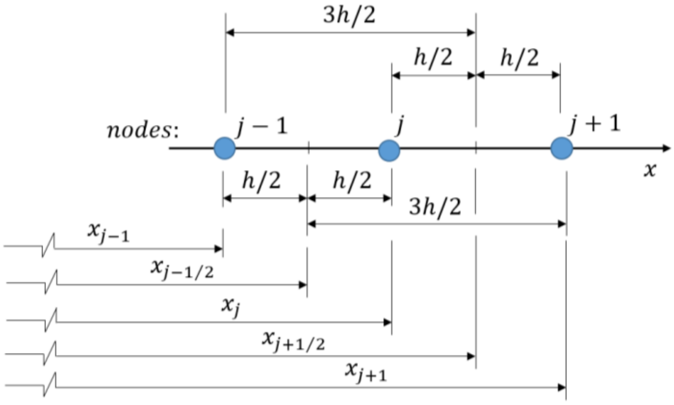

Figure 1. Unidimensional domain discretized by a finite difference grid of uniform spacing

The smallest portion of a discrete domain where it is possible to applicate the Simpson's 1/3 Rule consists of two discrete elements $[x_{j-1}, x_j]$ and $[x_j, x_{j+1}]$, both with length h as shown in Fig. 1. The integral I of a function $F(x)$ over these two elements is called single application of the Simpson's 1/3 Rule (Burden and Faires, 2011, Chapra and Canale, 2015):

$$I_{[x_{j-1},x_{j+1}]}^{Simpson} = \frac{(F_{j-1}+4F_j+F_{j+1})h}{3}, \tag{1}$$

with truncation error ε:

$$\varepsilon_{[x_{j-1},x_{j+1}]}^{Simpson} = -\frac{1}{90}F_{(\xi)}^{iv}h^5, \qquad x_{j-1} < \xi < x_{j+1}, \tag{2}$$

where F_{j-1}, F_j and F_{j+1} are discrete values of the function $F(x)$ to be integrated. They are assumed to be known at the nodal points x_{j-1}, x_j and x_{j+1}, respectively. The sub-indexes $j-1$ and $j+1$ means the adjacent points related to some generic point j on the uniformly spaced grid, as commonly named in the Finite Difference Method (FDM). In Eq. (2) $F_{(\xi)}^{iv}$ represents the fourth derivative of the function F at some point ξ somewhere in the open interval $]x_{j-1}, x_{j+1}[$. If the fourth-order derivative $F_{(\xi)}^{iv}$ is a function that varies with x, then the truncation error can only be estimated.

2. DEDUCTION OF THE TRUNCATION ERROR FOR A SINGLE APPLICATION OF THE SIMPSON'S 1/3 RULE

In the present work, the truncation equation is based on expansions in Taylor Series, instead of Interpolating Polynomials. Because of this, the truncation term will not be a single term calculated in an unknown position ξ, but a series where all terms are evaluated at the nodal point x_j. By truncating the number of terms of the series, it is possible to obtain the numerical error within a rounding error limit that can be known *a priori*, that is, calculated before conducting any numerical experiments.

The single application of the Simpson's 1/3 Rule requires the integration be made in two discrete intervals: $[x_{j-1}, x_j]$ and $[x_j, x_{j+1}]$. Also the expansion points need to be at the midpoint of each interval, conversely the integration formula is not attained. It began calculating the integral over both intervals and summing then to attain the integral of the overall interval:

$$I_{[j-1,j+1]}^{exact} = I_{[j-1,j]}^{exact} + I_{[j,j+1]}^{exact}. \tag{3}$$

2.1 Integration of $F(x)$ Expanded in Taylor Series Around $x_{j-1/2}$ and $x_{j+1/2}$

The dependent variable $F(x)$ is expanded in Taylor Series around the intermediary point $x_{j-1/2}$ as shown in Fig. 1 and the exact integral in the $[j-1,j]$ interval is given by:

$$I_{[j-1,j]}^{exact} = F_{j-1/2}h + \frac{2F_{j-1/2}^{ii}}{48}h^3 + \frac{2F_{j-1/2}^{iv}}{3840}h^5 + \frac{2F_{j-1/2}^{vi}}{645120}h^7 + \frac{2F_{j-1/2}^{viii}}{185794560}h^9 + \cdots \quad (4)$$

Calculating the exact integral in the $[j, j+1]$ interval by an expansion around the midpoint $x_{j+1/2}$ one can find:

$$I_{[j,j+1]}^{exact} = F_{j+1/2}h + \frac{2F_{j+1/2}^{ii}}{48}h^3 + \frac{2F_{j+1/2}^{iv}}{3840}h^5 + \frac{2F_{j+1/2}^{vi}}{645120}h^7 + \frac{2F_{j+1/2}^{viii}}{185794560}h^9 + \cdots \quad (5)$$

As stated by Eq. (3), the exact integral in the interval $[x_{j-1}, x_{j+1}]$ is the sum of Eq. (4) and Eq. (5), that is:

$$I_{[j-1,j+1]}^{exact} = (F_{j-1/2} + F_{j+1/2})h + \frac{2}{48}(F_{j-1/2}^{ii} + F_{j+1/2}^{ii})h^3 + \frac{2}{3840}(F_{j-1/2}^{iv} + F_{j+1/2}^{iv})h^5 + \frac{2}{645120}(F_{j-1/2}^{vi} + F_{j+1/2}^{vi})h^7 + \frac{2}{185794560}(F_{j-1/2}^{viii} + F_{j+1/2}^{viii})h^9 + \cdots \quad (6)$$

For now, Eq. (6) has only terms evaluated at the midpoints $x_{j-1/2}$ and $x_{j+1/2}$. The next step is calculating $F_{j-1/2}$, $F_{j+1/2}$ based on the function evaluated at the nodal points x_{j-1}, x_j and x_{j+1}.

2.2 Calculation of *I* Based on the Function Evaluated at Nodal Points

The function $F_{j-1/2}$ can be obtained by expanding the adjacent nodal points F_{j-1} and F_j around the point $x_{j-1/2}$. In the case of F_{j-1}, then $x_{j-1} - x_{j-1/2} = -h/2$, so one have:

$$F_{j-1} = F_{j-1/2} - \frac{F_{j-1/2}^{i}}{2}h + \frac{F_{j-1/2}^{ii}}{8}h^2 - \frac{F_{j-1/2}^{iii}}{48}h^3 + \frac{F_{j-1/2}^{iv}}{384}h^4 - \frac{F_{j-1/2}^{v}}{3840}h^5 + \frac{F_{j-1/2}^{vi}}{46080}h^6 - \frac{F_{j-1/2}^{vii}}{645120}h^7 + \frac{F_{j-1/2}^{viii}}{10321920}h^8 - \frac{F_{j-1/2}^{ix}}{185794560}h^9 + \cdots \quad (7)$$

In the case of F_j, considering $x_j - x_{j-1/2} = h/2$, one can find:

$$F_j = F_{j-1/2} + \frac{F_{j-1/2}^{i}}{2}h + \frac{F_{j-1/2}^{ii}}{8}h^2 + \frac{F_{j-1/2}^{iii}}{48}h^3 + \frac{F_{j-1/2}^{iv}}{384}h^4 + \frac{F_{j-1/2}^{v}}{3840}h^5 + \frac{F_{j-1/2}^{vi}}{46080}h^6 + \frac{F_{j-1/2}^{vii}}{645120}h^7 + \frac{F_{j-1/2}^{viii}}{10321920}h^8 + \frac{F_{j-1/2}^{ix}}{185794560}h^9 + \cdots \quad (8)$$

Summing Eq. (7) and Eq. (8) and isolating $F_{j-1/2}$:

$$F_{j-1/2} = \frac{F_{j-1}+F_j}{2} - \frac{F_{j-1/2}^{ii}}{8}h^2 - \frac{F_{j-1/2}^{iv}}{384}h^4 - \frac{F_{j-1/2}^{vi}}{46080}h^6 - \frac{F_{j-1/2}^{viii}}{10321920}h^8 - \cdots \quad (9)$$

To calculate $F_{j+1/2}$ a similar procedure is applied, but this time the Taylor Series expansion is around the midpoint $F_{j+1/2}$ and the functions to be expanded are F_j and F_{j+1}. This gives:

$$F_{j+1/2} = \frac{F_j+F_{j+1}}{2} - \frac{F_{j+1/2}^{ii}}{8}h^2 - \frac{F_{j+1/2}^{iv}}{384}h^4 - \frac{F_{j+1/2}^{vi}}{46080}h^6 - \frac{F_{j+1/2}^{viii}}{10321920}h^8 - \cdots \quad (10)$$

Substituting Eq. (9) and Eq. (10) in Eq. (6) removes the midpoint information in the term dependent of h:

$$I_{[j-1,j+1]}^{exact} = \frac{(F_{j-1}+2F_j+F_{j+1})}{2}h - \frac{4}{48}(F_{j-1/2}^{ii} + F_{j+1/2}^{ii})h^3 - \frac{8}{3840}(F_{j-1/2}^{iv} + F_{j+1/2}^{iv})h^5 - \frac{12}{645120}(F_{j-1/2}^{vi} + F_{j+1/2}^{vi})h^7 + \frac{16}{185794560}(F_{j-1/2}^{viii} + F_{j+1/2}^{viii})h^9 - \cdots \quad (11)$$

The next step is substituting the second order derivatives that appear in Eq. (11) by expressions of the function evaluated at the nodal points x_{j-1}, x_j and x_{j+1}.

2.3 Calculation of the Second Derivatives $F_{j-1/2}^{ii}$ and $F_{j+1/2}^{ii}$ Based on Values at the Nodal Points

In order to obtain $F^{ii}_{j-1/2}$ based on function values at the nodal points, it is necessary to obtain F_{j+1} expanded around the midpoint $x_{j-1/2}$. Looking at Fig. 1, one can see that $x_{j+1} - x_{j-1/2} = 3h/2$. This produces:

$$F_{j+1} = F_{j-1/2} + \frac{3F^{i}_{j-1/2}}{2}h + \frac{9F^{ii}_{j-1/2}}{8}h^2 + \frac{27F^{iii}_{j-1/2}}{48}h^3 + \frac{81F^{iv}_{j-1/2}}{384}h^4 + \frac{243F^{v}_{j-1/2}}{3840}h^5 + \frac{729F^{vi}_{j-1/2}}{46080}h^6 + \frac{2187F^{vii}_{j-1/2}}{645120}h^7 + \frac{6561F^{viii}_{j-1/2}}{10321920}h^8 + \cdots \quad (12)$$

Grouping Eq. (7), Eq. (8) and Eq. (12) gives the following linear system:

$$\begin{cases} F_{j-1} = F_{j-1/2} - \frac{F^{i}_{j-1/2}}{2}h + \frac{F^{ii}_{j-1/2}}{8}h^2 - \frac{F^{iii}_{j-1/2}}{48}h^3 + \frac{F^{iv}_{j-1/2}}{384}h^4 - \frac{F^{v}_{j-1/2}}{3840}h^5 + \frac{F^{vi}_{j-1/2}}{46080}h^6 - \cdots \\ F_{j} = F_{j-1/2} + \frac{F^{i}_{j-1/2}}{2}h + \frac{F^{ii}_{j-1/2}}{8}h^2 + \frac{F^{iii}_{j-1/2}}{48}h^3 + \frac{F^{iv}_{j-1/2}}{384}h^4 + \frac{F^{v}_{j-1/2}}{3840}h^5 + \frac{F^{vi}_{j-1/2}}{46080}h^6 + \cdots \\ F_{j+1} = F_{j-1/2} + \frac{3F^{i}_{j-1/2}}{2}h + \frac{9F^{ii}_{j-1/2}}{8}h^2 + \frac{27F^{iii}_{j-1/2}}{48}h^3 + \frac{81F^{iv}_{j-1/2}}{384}h^4 + \frac{243F^{v}_{j-1/2}}{3840}h^5 + \frac{729F^{vi}_{j-1/2}}{46080}h^6 + \cdots \end{cases} \quad (13)$$

Despite only terms of order lower or equal than six are shown in the Eq. (13), all terms until order eight are expanded and considered when solving the linear system for $F^{ii}_{j-1/2}$. The result is an equation where terms up to order six are deduced (note the division by h^2 to isolate $F^{ii}_{j-1/2}$). When $F^{ii}_{j-1/2}$ is isolated and substituted in Eq. (11) it produces an equation that shows terms up to order nine, therefore compatible with it. Obviously, the number of considered terms are choice of someone that intents to make *a priori* analysis. In this deduction, the authors choose to represent the truncation error with three terms.

The first and second terms in the right side of Eq. (13) are those need to be canceled in order to produce a series of order $\mathcal{O}(h)$. One can find real numbers X, Y and Z that multiplies, respectively, the first, second and third equation in the system (13):

$$\begin{bmatrix} 1 & 1 & 1 \\ -1/2 & 1/2 & 3/2 \\ 1/8 & 1/8 & 9/8 \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ C \end{bmatrix}, \quad C \neq 0\,. \quad (14)$$

Solving Eq. (14) for $C = 1$, gives: $X = 1$, $Y = -2$ and $Z = 1$. Multiplying each equation in system (13) for its respective constant and summing them, the second derivative $F^{ii}_{j-1/2}$ is found:

$$F^{ii}_{j-1/2} = \frac{F_{j-1} - 2F_j + F_{j+1}}{h^2} - \frac{24F^{iii}_{j-1/2}}{48}h - \frac{80F^{iv}_{j-1/2}}{384}h^2 - \frac{240F^{v}_{j-1/2}}{3840}h^3 - \frac{728F^{vi}_{j-1/2}}{46080}h^4 - \frac{2184F^{vii}_{j-1/2}}{645120}h^5 - \frac{6560F^{viii}_{j-1/2}}{10321920}h^6 - \cdots \quad (15)$$

In order to obtain $F^{ii}_{j+1/2}$, a similar development is required. It gives:

$$F^{ii}_{j+1/2} = \frac{F_{j-1} - 2F_j + F_{j+1}}{h^2} + \frac{24F^{iii}_{j+1/2}}{48}h - \frac{80F^{iv}_{j+1/2}}{384}h^2 + \frac{240F^{v}_{j+1/2}}{3840}h^3 - \frac{728F^{vi}_{j+1/2}}{46080}h^4 + \frac{2184F^{vii}_{j+1/2}}{645120}h^5 - \frac{6560F^{viii}_{j+1/2}}{10321920}h^6 + \cdots \quad (16)$$

Substituting Eq. (15) and Eq. (16) in the Eq. (11) gives:

$$I^{exact}_{[j-1,j+1]} = \frac{(F_{j-1} + 4F_j + F_{j+1})}{3}h + \frac{\left(F^{iii}_{j-1/2} - F^{iii}_{j+1/2}\right)}{24}h^4 + \frac{11\left(F^{iv}_{j-1/2} + F^{iv}_{j+1/2}\right)}{720}h^5 + \frac{\left(F^{v}_{j-1/2} - F^{v}_{j+1/2}\right)}{192}h^6 + \frac{157\left(F^{vi}_{j-1/2} + F^{vi}_{j+1/2}\right)}{120960}h^7 + \frac{13\left(F^{vii}_{j-1/2} - F^{vii}_{j+1/2}\right)}{46080}h^8 + \frac{307\left(F^{viii}_{j-1/2} + F^{viii}_{j+1/2}\right)}{5806080}h^9 + \cdots \quad (17)$$

One can see the first term in the right side of Eq. (17) is the approximation called Simpson's 1/3 Rule, but the next terms needs to be written in the nodal point x_j for the equation to be useful. The last step is the expansion of all derivatives around the nodal point x_j.

2.4 Expansion of the Derivatives Around the Central Nodal Point x_j

Beginning with derivatives of order three $F_{j-1/2}^{iii}$ and $F_{j+1/2}^{iii}$, they can be expanded around the nodal point x_j. Note that there is no need to expand the series beyond order five to result in terms of order nine when replacing them in the Eq. (17):

$$F_{j-1/2}^{iii} = F_j^{iiii} - \frac{F_j^{iv}}{2}h + \frac{F_j^{v}}{8}h^2 - \frac{F_j^{vi}}{48}h^3 + \frac{F_j^{vii}}{384}h^4 - \frac{F_j^{viii}}{3840}h^5 + \cdots \quad (18)$$

$$F_{j+1/2}^{iii} = F_j^{iiii} + \frac{F_j^{iv}}{2}h + \frac{F_j^{v}}{8}h^2 + \frac{F_j^{vi}}{48}h^3 + \frac{F_j^{vii}}{384}h^4 + \frac{F_j^{viii}}{3840}h^5 + \cdots \quad (19)$$

Derivatives of order four $F_{j-1/2}^{iv}$ and $F_{j+1/2}^{iv}$ up to the derivatives of order eight $F_{j-1/2}^{viii}$ and $F_{j+1/2}^{viii}$ are:

$$F_{j-1/2}^{iv} = F_j^{iv} - \frac{F_j^{v}}{2}h + \frac{F_j^{vi}}{8}h^2 - \frac{F_j^{vii}}{48}h^3 + \frac{F_j^{viii}}{384}h^4 - \cdots \quad (20)$$

$$F_{j+1/2}^{iv} = F_j^{iv} + \frac{F_j^{v}}{2}h + \frac{F_j^{vi}}{8}h^2 + \frac{F_j^{vii}}{48}h^3 + \frac{F_j^{viii}}{384}h^4 + \cdots \quad (21)$$

$$F_{j-1/2}^{v} = F_j^{v} - \frac{F_j^{vi}}{2}h + \frac{F_j^{vii}}{8}h^2 - \frac{F_j^{viii}}{48}h^3 + \cdots \quad (22)$$

$$F_{j+1/2}^{v} = F_j^{v} + \frac{F_j^{vi}}{2}h + \frac{F_j^{vii}}{8}h^2 + \frac{F_j^{viii}}{48}h^3 + \cdots \quad (23)$$

$$F_{j-1/2}^{vi} = F_j^{vi} - \frac{F_j^{vii}}{2}h + \frac{F_j^{viii}}{8}h^2 - \cdots \quad (24)$$

$$F_{j+1/2}^{vi} = F_j^{vi} + \frac{F_j^{vii}}{2}h + \frac{F_j^{viii}}{8}h^2 + \cdots \quad (25)$$

$$F_{j-1/2}^{vii} = F_j^{vii} - \frac{F_j^{viii}}{2}h + \cdots \quad (26)$$

$$F_{j+1/2}^{vii} = F_j^{vii} + \frac{F_j^{viii}}{2}h + \cdots \quad (27)$$

$$F_{j-1/2}^{viii} = F_j^{viii} - \cdots \quad (28)$$

$$F_{j+1/2}^{viii} = F_j^{viii} + \cdots \quad (29)$$

Substituting Eq. (18) to Eq. (29) in the Eq. (17) and simplifying the terms:

$$I_{[j-1,j+1]}^{exact} = \frac{(F_{j-1}+4F_j+F_{j+1})}{3}h - \frac{1}{90}F_j^{iv}h^5 - \frac{1}{1890}F_j^{vi}h^7 - \frac{1}{90720}F_j^{viii}h^9 - \cdots \quad (30)$$

From Eq. (30) is extracted the single application of the Simpson's 1/3 Rule $I_{[j-1,j+1]}^{Simpson}$:

$$I_{[j-1,j+1]}^{Simpson} = \frac{(F_{j-1}+4F_j+F_{j+1})}{3}h\,. \quad (31)$$

The remaining terms constitute the truncation error $\varepsilon_{[j-1,j+1]}^{Simpson}$:

$$\varepsilon_{[j-1,j+1]}^{Simpson} = -\frac{1}{90}F_j^{iv}h^5 - \frac{1}{1890}F_j^{vi}h^7 - \frac{1}{90720}F_j^{viii}h^9 - \cdots \quad (32)$$

Note that the first term in the right side of Eq. (32) has the same order of accuracy and same coefficient that Eq. (2). The difference is that the fourth order derivative is evaluated at the nodal point x_j instead of an unknown point ξ. Other difference between them is that Eq. (2) is a single term equation calculated in an unknown position while Eq. (32) constitutes a series calculated in a known position.

Based on Eq. (32), one can find that the single application of the Simpson's 1/3 Rule has the asymptotic term of order five and the following terms are of odd orders. The true orders p_m are:

$$p_m = 5, 7, 9, \ldots \tag{33}$$

3. TRUNCATION ERROR FOR THE COMPOSITE APPLICATION OF THE SIMPSON'S 1/3 RULE

Once the error equation is deduced for two discrete intervals, now it is extended to a large domain $[a, b]$ of length $L = b - a$ that should be divided in an even number of intervals. Assuming a domain arbitrarily divided into $N = 6$ intervals, then the seven points are numbered as $P = 0, 1, 2, 3, 4, 5, 6$ as shown in Fig. 2.

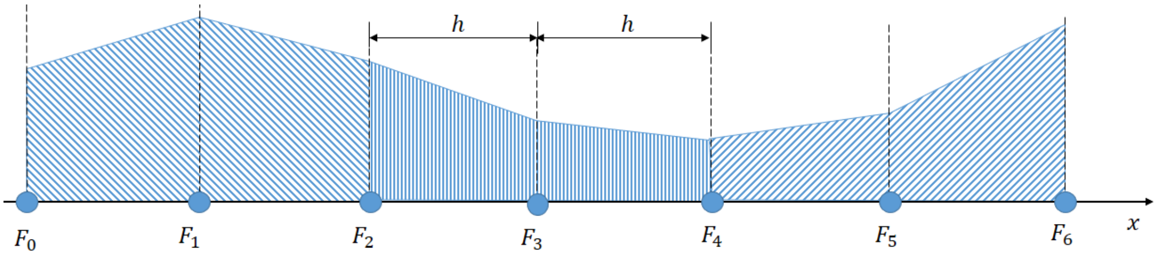

Figure 2. Hypothetical domain discretized with six intervals

The composite application of the Simpson's 1/3 Rule derived based on interpolating polynomials is given by Chapra and Canale (2015):

$$I_L^{exact} = \frac{h}{3}\left[F_0 + 4\sum_{j=1,3,5,\ldots}^{N-1}(F_j) + 2\sum_{j=2,4,\ldots}^{N-2}(F_j) + F_N\right] - \frac{(b-a)}{180}F_\mu^{iv}h^4, \quad a < \mu < b\,, \tag{34}$$

where the first term in the right side is the approximation called composite Simpson's 1/3 Rule and the second term is its truncation error, where the exact position of μ is not known, except by the fact it is located inside the integration interval.

The composite Simpson's 1/3 Rule also can be written in a more convenient way:

$$I_L^{Simpson} = \sum_{j=1,3,5,\ldots}^{N-1}(F_{j-1} + 4F_j + F_{j+1})\frac{h}{3}, \tag{35}$$

as easily seen by considering the hypothetical case shown in Fig. 2:

$$I_L^{Simpson} = [(F_0 + 4F_1 + F_2) + (F_2 + 4F_3 + F_4) + (F_4 + 4F_5 + F_6)]\frac{h}{3}.$$

Considering the analytical integral over the domain, one can write, based on Eq. (30) and Eq. (35):

$$I_L^{exact} = \int_a^b F_{(x)}dx = \sum_{j=1,3,5,\ldots}^{N-1}\frac{(F_{j-1}+4F_j+F_{j+1})}{3}h + \sum_{j=1,3,5,\ldots}^{N-1}\left[-\frac{1}{90}F_j^{iv}h^5 - \frac{1}{1890}F_j^{vi}h^7 - \frac{1}{90720}F_j^{viii}h^9 - \cdots\right]. \tag{36}$$

While the first term in the right side of Eq. (36) represents the composite application of the Simpson's 1/3 Rule, the second term represents its truncation error $\varepsilon_L^{Simpson}$:

$$\varepsilon_L^{Simpson} = -\frac{1}{90}\sum_{j=1,3,5,\ldots}^{N-1}F_j^{iv}\,h^5 - \frac{1}{1890}\sum_{j=1,3,5,\ldots}^{N-1}F_j^{vi}\,h^7 - \frac{1}{90720}\sum_{j=1,3,5,\ldots}^{N-1}F_j^{viii}\,h^9 - \cdots \tag{37}$$

Defining the following averages of the derivatives of orders four, six and eight:

$$\overline{F_j^{iv}} = \frac{\sum_{j=1,3,5,\ldots}^{N-1}F_j^{iv}}{(N/2)}, \quad \overline{F_j^{vi}} = \frac{\sum_{j=1,3,5,\ldots}^{N-1}F_j^{vi}}{(N/2)}, \quad \overline{F_j^{viii}} = \frac{\sum_{j=1,3,5,\ldots}^{N-1}F_j^{viii}}{(N/2)}, \tag{38}$$

substituting them in the Eq. (37) and evidencing the N and one h of each term gives:

$$\varepsilon_L^{Simpson} = -Nh\left(\frac{1}{180}\overline{F_j^{iv}}h^4 + \frac{1}{3780}\overline{F_j^{vi}}h^6 + \frac{1}{181440}\overline{F_j^{viii}}h^8 + \cdots\right). \tag{39}$$

Knowing that $h = L/N$, then $L = Nh$, so Eq. (39) can be rewritten as:

$$\varepsilon_L^{Simpson} = -\frac{L}{180}\overline{F_j^{iv}}h^4 - \frac{L}{3780}\overline{F_j^{vi}}h^6 - \frac{L}{181440}\overline{F_j^{viii}}h^8 - \cdots \quad (40)$$

Comparing Eq. (40) with its counterpart deduced by using the classical integration of interpolating polynomials Eq. (34) (last term in the right side), one can see they are similar, except by the fact Eq. (34) has its derivative evaluated at some point μ of unknown position inside the domain and Eq. (40) has all its derivatives evaluated at every odd nodal point. In addition, it has many terms as its number of non-null derivatives. Comparing Eq. (40) with Eq. (32) it is obvious the order reduction. All orders reduce one unity, thus the integral over the entire domain when using the Simpson's 1/3 Rule produces the true orders:

$$p_m = 4, 6, 8, \ldots \quad (41)$$

Equation (32), Eq. (33), Eq. (40) and Eq. (41) constitute the main results of this work.

4. DEFINITION OF THE TEST PROBLEMS

A way to demonstrate the correctness of Eq. (40) and Eq. (41) is by measuring the numerical error resulting from the integration of polynomials. As higher is the order of the polynomial, more terms of Eq. (40) are non-null. The test problems chosen are:

$$I = \int_2^5 x^n \, dx \, , \quad (42)$$

where $n = 3, 4, 5, 6, 7, 8, 9$. The limits of integration are arbitrarily chosen, avoiding the classical $L = 1$ interval of integration (in fact, the authors recommend that in verification studies, none of the variables assume values 0 or 1, because they are neutral elements for addition and multiplication, respectively). To test a problem for which the number of terms in Eq. (40) is infinite, the authors include the integral of the exponential function over the same interval:

$$I = \int_2^5 e^x \, dx \, . \quad (43)$$

The problems are labeled in Tab. 1 and classified according to the null and non-null average derivatives appearing in Eq. (40). Based in Eq. (40), Tab. 1 shows that the integration of a cubic function by the 1/3 Simpson's Rule is exact, as well known. As the degree of the polynomial increases, more terms are added as non-null contributions to the truncation error. Polynomials of degrees 4 and 5 have only the first non-null term in Eq. (40), polynomials of degree 6 and 7 has the first and second terms, and so on. Note that Eq. (40) presents exact value for the truncation error of polynomials up to degree 9. The integration of polynomials of higher degrees are not exact, but as the grid element size tends to zero, the calculated value tends to zero with order-of-accuracy 10.

Table 1. Average derivatives that appear in Eq. (40) for each test problem

$problem$	$\int (\,)dx$	$average\ derivative \neq 0$	$average\ derivative = 0$
A	x^3		$\overline{F^{iv}}, \overline{F^{vi}}, \overline{F^{viii}}$
B	x^4	$\overline{F^{iv}}$	$\overline{F^{vi}}, \overline{F^{viii}}$
C	x^5	$\overline{F^{iv}}$	$\overline{F^{vi}}, \overline{F^{viii}}$
D	x^6	$\overline{F^{iv}}, \overline{F^{vi}}$	$\overline{F^{viii}}$
E	x^7	$\overline{F^{iv}}, \overline{F^{vi}}$	$\overline{F^{viii}}$
F	x^8	$\overline{F^{iv}}, \overline{F^{vi}}, \overline{F^{viii}}$	
G	x^9	$\overline{F^{iv}}, \overline{F^{vi}}, \overline{F^{viii}}$	
H	e^x	$\overline{F^{iv}}, \overline{F^{vi}}, \overline{F^{viii}}, \ldots$	

5. RESULTS

All results presented in this work come from a program written in FORTRAN95 language. It makes all computations using real-type variables and constants as quadruple precision. However, the analytical solutions of Eq. (40), Eq. (42) and

Eq. (43) are calculated with 50 significant digits with the software MAPLE 17. The first 34 are directly written in the FORTRAN program to guarantee analytical solutions I_L^{exact} more accurate than the numerical solutions $I_L^{Simpson}$.

All problems are solved in 14 grids with n from 2 to 16,384 elements. Table 2 presents the comparison between analytical and numerical results for all problems in the 1,024 grid, which is considered a sufficiently fine grid. Analytical values are presented with few decimal digits if they have a finite number of decimal digits.

The last two columns in Tab. 2 represent the truncation error $\varepsilon_L^{Simpson}$ predicted by Eq. (40) and its relative value $E(\%)$, defined by Eq. (44). As the $\varepsilon_L^{Simpson}$ values are rounded-off with two significant digits, then I_L^{exact} and $I_L^{Simpson}$ are rounded-off accordingly.

$$E(\%) = 100\frac{\varepsilon_L^{Simpson}}{I_L^{exact}}. \tag{44}$$

One can observe in Tab. 2 that the analytical solution of the problems from A to G is obtained when the numerical solution $I_L^{Simpson}$ is summed to its respective predicted error $\varepsilon_L^{Simpson}$. This behavior is not verified only in problem H, because the exponential function has infinite derivatives, and only three terms are deduced in Eq. (40).

Table 2. Comparison between calculated and measured relative error for the 1,024 grid

$Problem$	I_L^{exact}	$I_L^{Simpson}$	$\varepsilon_L^{Simpson}$	$E(\%)$
A	152.25	152.25	0.0E+00	0.0E+00
B	618.6	618.600000000029	-2.9E-11	-4.8E-14
C	2,593.5	2,593.50000000052	-5.2E-10	-2.0E-13
D	11,142.4285714286	11,142.4285714343	-5.7E-09	-5.2E-13
E	48,796.125	48,796.125000052	-5.2E-08	-1.1E-12
F	216,957.0	216,957.00000043	-4.3E-07	-2.0E-10
G	976,460.1	976,460.1000032	-3.2E-06	-3.3E-10
H	141.024103003644…	141.024103003704	-5.8E-11	-4.1E-11

The difference between the error calculated with the three terms of Eq. (40) and the error measured are shown in Tab. 3 for all problems. It is interesting to note that the magnitude of the errors difference $\Delta\varepsilon$ for problem H is about the same magnitude as other problems, at least for the grid of 1,024 elements.

The results presented from Tab. 1 up to Tab. 3 are without employing error-improving techniques, as Repeated Richardson Extrapolation (RRE). When RRE is used, the truncation error can be greatly reduced, attaining a more accurate numerical solution (Roache, 2009, Roache and Knupp, 1993, Marchi et al., 2013). The technique is applied in this work not with the objective of improving accuracy, but as a way to demonstrate the correctness of Eq. (41), by showing through numerical experiments that the orders predicted by Eq. (41) are attained as the extrapolations are carry out.

Table 3. Comparison between calculated and measured error for the 1,024 grid

$Problem$	ε *a priori* (Eq. 40)	ε *a posteriori*	$\Delta\varepsilon$
A	0.0E+00	0.0E+00	0.0E+00
B	-2.9E-11	-2.9E-11	-2.0E-32
C	-5.2E-10	-5.2E-10	0.0E+00
D	-5.7E-09	-5.7E-09	6.8E-31
E	-5.2E-08	-5.2E-08	0.0E+00
F	-4.3E-07	-4.3E-07	0.0E+00
G	-3.2E-06	-3.2E-06	1.2E-28
H	-5.8E-11	-5.8E-11	2.8E-31

Figure 3 shows the typical behavior of the application of the RRE based on the apparent order (Marchi et al., 2013) for the integral of the exponential function. The data set named "0" means the numerical error results are obtained in the 14 grids without RRE. This set reaches errors in the order of 10^{-15} in the finest grid and has fourth order-of-accuracy, as can be noted by the inclination of the results in the log versus log scale. After one Richardson Extrapolation, the order increases to 6, as observed in the second data set, and so on. In the lower portion of the Fig. 3, the tenth and twelfth orders suffer the influence of the round-off error as expected, because the magnitude of the error is near the limit of the quadruple precision computation. The extrapolation level "5" is completely polluted with round-off error.

The apparent or observed order (Roache, 2009) is the measurement of how much the error reduces as the grid element size is reduced. Details of its calculation when using RRE are found in Marchi et al. (2013). In graphical form, it is represented in Fig. 4, where one can see that the orders predicted by *a priori* analysis (Eq. (41)) are confirmed by *a posteriori* experiments for all grids without round-off error influence.

The results for the polynomial functions are similar to those presented for the integral of the exponential function, but as they have a finite number of non-null derivatives, after a sufficient number of extrapolations, the analytical solution is attained numerically, thus the next extrapolated solutions do not change, and the observed order concept loses validity.

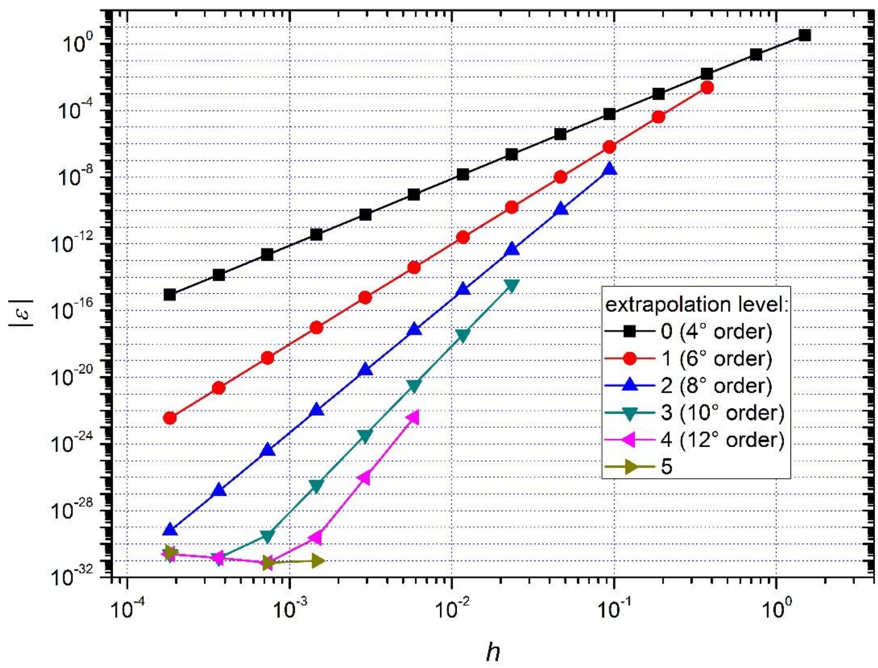

Figure 3. Module of the truncation error for the integral of e^x as function of the grid element size

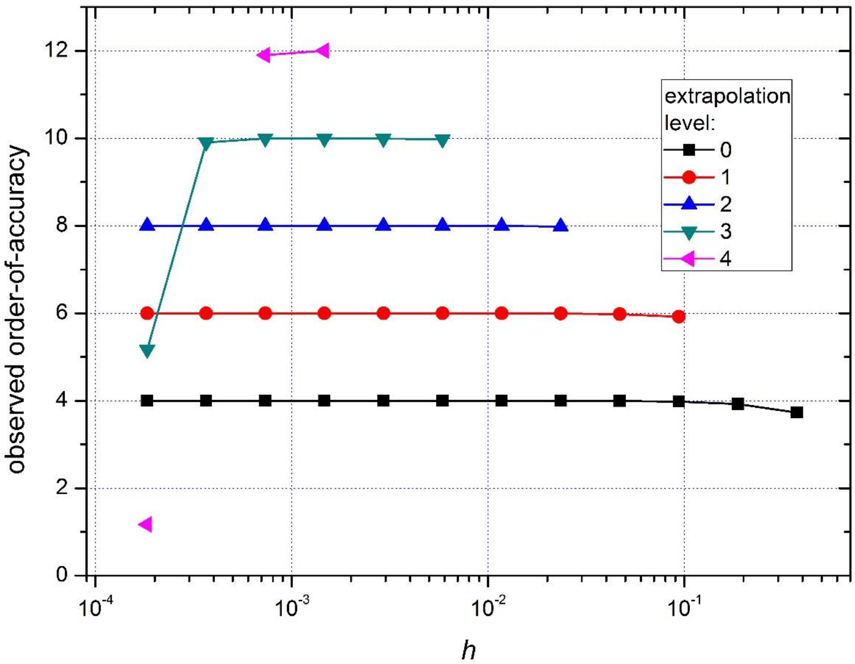

Figure 4. Observed Orders for the integration of e^x as function of the element grid size

6. CONCLUSION

This paper presents a deduction of the truncation error for the Simpson's 1/3 Rule integration formula. Represented by Eq. (40), the truncation error equation is based on Taylor Series expansions evaluated at nodal points of a grid of Finite Differences. The representation has infinite terms, and the predicted true orders are $4, 6, 8, \ldots$, thus the asymptotic order is 4 and the subsequent orders present difference of 2 orders between them.

Although the deduction is not formally proved, *a posteriori* procedure is conducted to shown the correctness of the error equation. The most convincing test is the comparison between the calculated and measured errors, where all polynomials reach the analytical result when numerically calculated (with some round-off error consistent with the precision of the real-type variables).

Despite the use of Eq. (40) is not so practical, the procedure of observing the apparent orders as stated by Eq. (41) is relevant to code and solution verification activities, especially when RRE is also used.

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