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Validating Explicit Third Order Euler Technique for Reactor Design and Exponential Growth Problems

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Abstract

The purpose of this present paper is to validate an explicit third order Euler approximation technique for reactor design and exponential growth problems. The computation results reveal that the numerical solution obtained by explicit third order Euler method is better in comparison with analytical solution due to simple improvement carried out in the employed method. The advantage of employing explicit third order Euler method is consistent, stable, efficient, accurate, convergent order is 3, wider region of absolute stability and easy to implement with lower computational cost.

Keywords: Exponential growth, reactor design, explicit third order Euler method, ordinary differential equations, initial value problems

Introduction

It is well known from literature study that differential equations appear in many areas of science and engineering. The basic principle of mathematical science is that, in order to solve a new problem, reduce it into a problem that has already been solved. Moreover, many linear and nonlinear problems in engineering and science can be considered as a mathematical problem especially in the form of differential equation. An equation involving a function and its derivative is called a differential equation. Many differential equations cannot be solved analytically; however, in science and engineering, a numeric approximation to the solution is often good enough to solve a problem. It is significant to point out that, many nonlinear differential equations take place in applied and engineering sciences such as physics, solid state physics, astrophysics, nuclear physics, astronomy, fluid mechanics, chemistry, hydrodynamic, including long wave and chemical reaction-diffusion models, aircraft dynamics and so on. It is true to state that developments in computer science and technology have allowed for solutions of nonlinear problems through existing or new numerical methods and algorithms.

Furthermore, it is evident that, the Euler method is simple one-step method to solve IVPs. It employs only one piece of information from the past and evaluates the driving function only once per step. For computational purposes, Euler technique is not advisable because a considerable effort is required to improve accuracy but in case of third order Euler method a better result can be obtained. In spite of its limitations, Euler method [1,2] remains to be a basic building block for higher accuracy methods, for instance Runge-Kutta or Linear Multistep methods etc. Since the difference equation is linear in y_n and f_n and being a one-step method, it can easily handle initial value problems (IVPs) that require variable step-size. It was noticed by Runge [3], that sometimes Euler's technique gives rise to a rather inefficient approximation of the integral by the area of a rectangle of height $f(x_0)$.

In most cases, nonlinear problems do not admit analytical solution, so the associated equations should be solved using special known techniques or by novel methods. Recently, much attention has been dedicated to newly developed techniques and algorithms to construct an analytic solution of the equations. It is always better to obtain exact solution for the given differential equations but, due to some complications like time consumption and more manual operations it is not possible to find analytical solutions for such mathematical problems. Therefore, it is necessary to approximate (numerical) solutions. There are some numerical techniques existing for solving such differential equation such as Euler's method, Pointwise method, Picards method, Improved Euler's method, Power Series method, Modified Euler's method, Predictor Corrector method, Taylor's method, Runge-Kutta second and fourth order method, etc. Runge-Kutta (RK) techniques have become very popular and efficient toll for computational purpose due to many application problems are solved effectively. Particularly RK algorithms are adapted to solve differential equations efficiently that are equivalent to approximate the exact solutions by matching 'n' terms of the Taylor series expansion. Akanbi [4] introduced a third order Euler technique for solving IVPs with detailed discussion on including development and analysis, stability, absolute stability and convergence etc. In this article, third order Euler approximation technique is implemented to achieve better results for reactor design and exponential growth problems. A detailed discussion on obtaining error control both local truncation error and global truncation error for new RK fourth order embedded means (heronian and root square) is given by Senthilkumar [5] to solve the real time application problems in image processing under cellular nerural network environment efficiently. The rest of the paper is organized as follows. In section 2, a short note on third order Euler method is discussed including pseudo code. Section 3 deals with two different problems such as reactor design, exponential growth problems, IVPs and its corresponding numerical results. Finally, conclusion is given in section 4.

A short note on third order Euler method

As pointed out by Butcher [6], that there are many different techniques which can be employed to approximate solutions to a differential equation if ODE does not have an exact solution or solution is difficult to find. It is known, that numerical solution of ordinary differential equation is the most vital method ever developed in continuous time dynamics. Because most ordinary differential equations are not soluble analytically, hence, numerical integration is the only way to yield information about the trajectory. Many different techniques have been introduced and employed in an attempt to solve accurately, various types of ODEs. But, all these, discretise the differential system, to produce a difference equation or map [7]. The techniques attain dissimilar maps from the same equation, but they have the similar aim; that the dynamics of the maps, should correspond closely, to the dynamics of the differential equation. Indeed, with the advent of modern digital computers, numerical techniques are now an increasingly attractive and efficient way to obtain approximate solutions to differential equations that had hitherto proved difficult, even impossible to solve analytically [8]. The investigation of differential equations has three major facets such as analytical / exact / symbolic methods, geometric methods and numerical methods. It is important to point out that most ordinary differential equations cannot be solved exactly therefore, it is essential to employ geometric and numerical methods [9,10]. It is known that, most of the differential equations can be solved efficiently by any one of the existing numerical methods or through newly developed techniques. Graphical methods describe how the solutions to a differential equation behave, for instance, in the presence of funnels [11-14].

Let us consider a first-order ODE is of the form;

$$y'(x) = f(x, y) \tag{1}$$

However, the general form of an Initial Value Problems (IVPs) related with this model is;

$$y'(x) = f(x, y),\ y(x_0) = \eta \tag{2}$$

where $x \in \mathbb{R}$; $y, \eta \in \mathbb{R}^n$ and $f: \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ when f does not depend explicitly on x, Eq. (1) is called as autonomous system [15]. An approximate solution to an IVP Eq. (1) is typically achieved by iterating a set of difference equations that approximate the original system. According to Euler computing a discrete set { }, for arguments { }, using the difference equation $y_{n+1} - y_n = hf(x_n, y_n)$, n= 1, 2, … m, where the step-length $h = x_{n+1} - x_n$ is ease [16,17]. Also, in Euler method, y_{n+1} depends explicitly on y_n but on no earlier of y_n, y_{n-1}, … The function f is evaluated only once in the step from the computation of y_n to the computation of y_{n+1}; Moreover, only the function f itself is used rather than f_2, f_3, ... say which yield values of $y''(x)$, $y'''(x)$, in terms of $y(x)$ or of f' (the Jacobian of f), f'', ….

Euler technique is both one-step and multi-step, and because of this fact together with the stability requirements, can mean that the step-length h has to be chosen to be very small and as noted in [1,2]. Further, "the method of Euler is ideal as an object of theoretical study but unsatisfactory as a means of obtaining accurate results". Owing to the low accuracy and poor stability behaviour, generalizations have been made to the method of Euler.

The most important generalizations of Euler equations are [18]:

(a) The use of formulae that violate (i). That is, y_{n+1} depends on y_{n-1}, …, y_{n-k} ($k \geq 1$) as well as on y_n. These methods are known as linear multistep methods;

(b) The use of formulae that violates (ii). That is more than one evaluation of f is involved in a formula for y_{n+1}. These methods are known as Runge-Kutta methods (and include methods such as mid-point quadrature rule and trapezoidal method).

(c) The use of formulae that violate (iii). For example, expressions for $y''(x)$, $y'''(x)$, … may be used along with an expression for $y'(x)$. The Taylor series method is an example of such a method [19].

In general, the percentage of error can be computed using the following formula as;

$$percentage\ of\ error = \frac{|true\ solution - approximate\ solution|}{true\ solution} \times 100 \tag{3}$$

Pseudo code for explicit third order Euler method

Step 1: define $f(x,y)$

Step 2: input x_n and y_n.

Step 3: input step-size, h and the number of steps, n.

Step 4: for j from 1 to n do

Step 4.1: $m = f(x_n, y_n)$

Step 4.2: $y_{n+1} = y_n + hf\left(x_n + \frac{h}{2}, y_n + \frac{h}{2} f\left(x_n + \frac{h}{2}, y_n + \frac{h}{3} f(x_n, y_n)\right)\right)$

Step 4.3: print x_n and y_n

Step 4.4: $x_n = x_{n+1}$

Step 4.5: $y_n = y_{n+1}$

Step 5: end

and the corresponding stability polynomial is $R(Z) = 1 + z + \frac{z^2}{2} + \frac{z^3}{6}$, which possesses wider region of absolute stability. The test of convergence and stability function also reveals that the method is of order 3 [4]. It is known that, the quality of the numerical solution depends on the step-size (h). In order to analyse any numerical methods for ODEs, consistency, stability and convergence are important factors. For stability, a scheme is unstable if it produces exponentially growing solutions for a problem for which the exact solution is bounded. Usually, stability introduces restrictions on the step-length (h). In case of region of stability, the range of $h\lambda$ for which the selected method is stable. Furthermore, in case of convergence, the numerical solution converges to the exact solution if the scheme is consistent and stable.

A numerical reactor design problem

The investigation of given nonlinear problems is of crucial importance, not only in all areas of mathematical physics, physics, astronomy, oceanography etc. but also in engineering and other disciplines, since most phenomena in our real world are essentially nonlinear and are described by nonlinear equations. It is very difficult to solve nonlinear problems and, in general, it is frequently more difficult to yield an analytical approximation solution than a numerical one for a given nonlinear problem.

Apply third order Euler method with a step length of 0.1, to determine how large the reactor must be if a conversion of 80 % is desired. Let us consider a reactor design problem for building a reactor which will be employed to carry out this reaction such that the elementary liquid-phase reaction A tends to B is to be carried out in an isothermal, isobaric plug flow reactor (PFR) at 30 °C. The feed enters at a concentration of 0.25 mol/L and at a rate of 3 mol/min. The reaction constant is known experimentally to be 0.01 min^{-1} at this temperature.

It is essential to simplify the reactor design equation which is of the form;

$$\frac{dV}{dX} = \frac{F_{Ao}}{kC_{Ao}(1-X)} \tag{4}$$

The following equation can be obtained by Lumping the given flow, concentration, and reaction constant together;

$$\frac{dV}{dX} = 1200\frac{1}{1-X} \tag{5}$$

Because, no volume is needed for a conversion of zero, the initial condition needed is V(0) = 0.

In simple, $V_{i+1} = V_i + 1200 \times 0.05 \times \dfrac{1}{1-X}$ (6)

Table 1 Comparison between exact and numerical solution for reactor design problem.

Time (t)	Exact solution	Numerical solution
0.00	0	0
0.10	126.4326	126.432
0.20	267.7723	267.772
0.30	428.0099	428.009
0.40	612.9907	612.990
0.50	831.7766	831.776
0.60	1099.549	1099.549
0.70	1444.767	1444.767
0.80	1931.325	1931.325

Exponential growth: Under exponential type constrained growth of biological organisms, positive feedback electrical systems, and chemical reactions generating their own catalyst problems can be encountered.

$$\frac{dy}{dt} = \lambda y \text{ with solution } y(t) = y_0\, e^{\lambda t} \tag{7}$$

An example for a simple growth ODE

Finding numerical solution by consider the following $\frac{dy}{dt} = 2.77259y$ with y(0) = 1.00;

Solution is y = exp(+2.773 x) = 16^x. (8)

Table 2 Comparison between exact and numerical solution for exponential growth problem.

Time (t)	Exact solution	Numerical solution
0.000	1.000	1.00
0.125	1.414	1.42
0.250	2.000	1.99
0.375	2.828	2.85
0.500	4.000	3.99
0.625	5.657	5.75
0.750	8.000	7.98
0.875	11.31	11.45
1.000	16.00	15.95

Numerical problem and results

Let us consider a simple initial value problem $y' = 2 - e^{-4t} - 2y; y(0) = 1$ to compute approximate solution using explicit third order Euler approximation technique. The analytical solution is given by;

$$y(x) = 1 + \frac{1}{2}e^{-4t} - \frac{1}{2}e^{-2t} \tag{9}$$

Table 3 Comparison between exact and numerical solution for initial value problem.

Time (t)	Exact solution	Numerical solution
0.00	1.0000	1.0000
0.10	0.925794646	0.925794
0.20	0.889504459	0.889504
0.30	0.87619128	0.876191
0.40	0.876283777	0.876283
0.50	0.883727921	0.883727

Numerical techniques employ exact algorithms to present numerical solutions to linear or nonlinear mathematical problems. On contradictory, analytic techniques employ exact theorems to present formulas that can be used to present numerical solutions to mathematical problems with or without the use of numerical techniques. Numerical solutions very rarely can contribute to proofs of novel notions. Analytic solutions are generally considered to be "stronger". It is imperative to mention that, up to some extend the numerical solution matches with the exact solution (see **Table 1 - 3**). In case of numeric solution, if h, is small one can obtain almost equivalent to exact solution but takes more time to complete its task.

Conclusions

In this paper, a different attempt to solve reactor design, exponential growth problem and initial value problem is carried out using an explicit third order Euler approximation technique. The benefit of incorporating explicit third order Euler method is consistent, stable, efficient, accurate, convergent order is 3, wider region of absolute stability and easy to implement with lower computational cost. It is noticed that the numerical solution obtained through explicit third order Euler method is better in comparison with analytical solution.

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