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Developing Clean Technology through Approximate Solutions of Mathematical Models

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Abstract

In this paper, the role of mathematical modeling in the development of clean technology has been considered. One method each for obtaining approximate solutions of mathematical models by ordinary differential equations and partial differential equations respectively arising from the modeling of systems and physical phenomena has been considered. The construction of continuous hybrid methods for the numerical approximation of the solutions of initial value problems of ordinary differential equations as well as homotopy analysis method, an approximate analytical method, for the solution of nonlinear partial differential equations are discussed.

Key words: *Mathematical models, simulation, continuous hybrid methods, homotopy analysis method*

1. Introduction

The term "clean technologies" refer to production systems developed and adopted for the primary purpose of improving environmental performance, (Kolturiewicz, 2008). The development of these environmentally friendly technologies is of great interest to scientists and governments all over the world as a result of the effects of global warming. In Nigeria for instance, a Science and Technology Policy, which advocates the use of clean technologies in production systems, was launched in 2011 by her federal government to underscore the importance it accords the development of clean technologies (Federal Republic of Nigeria Science Technology and Innovation Policy, September, 2011).

The reality is that this advancement in technology has modified in many ways the expectations facing mathematicians and the practice of applied research. With industries becoming typically "high-tech", computationally intensive methods are employed at all levels. The increased supply in computing power has also made it possible to implement and apply computational methods no matter how sophisticated. This interplay of mathematics, computing and technology could best be described as the art of mathematical modeling and simulation (Hellio, 2009).

According to the report of the 2012 Workshop on mathematical modeling and simulation of power plant and CO_2 capture held at the University of Warwick, mathematical modeling and simulation play important roles in proof of concept, feasibility study, reliability and performance analysis for the designs and development of new systems to be cost effective and robust. This is especially relevant where experiments with real objects are difficult or completely not feasible.

The design and development of any new system, typically begins with a mathematical model which is assumed to represent the structure and the laws governing the system or phenomenon. The model represents the key relationships among system components by means of equations. The equations can be derived in a number of ways. Many of them come from extensive scientific studies that have formulated and tested mathematical relationship against real data. Some come from laboratory testing of relationships where that is feasible. Sometimes real data are used to derive relationships using statistical techniques to fit a particular relationship to the data and to measure the level of error associated with that representation.

The aim of this paper is not to build mathematical models but to discuss the numerical approximation to the solutions of the mathematical models of systems that lead to differential equations.

The paper is arranged as follows: In section two mathematical models by ordinary differential equations and the methods of obtaining approximate solutions are considered; models by partial differential equations and the methods of approximating their solutions are described as well in section three; and section four is the conclusion

2. Models by Ordinary Differential Equations (ODE)

Many mathematical problems in applied mathematics lead to ordinary differential equations. In the simplest case, to solve ODE one seeks a differentiable function, say $x=x(t)$ of one real variable t, whose n^{th} derivative, $x^n(t)$, $n=1,2,\ldots,n-1$, is to satisfy an equation of the form

$$\frac{d^n x}{dt^n}=f\left(t,x(t),x^1(t),x^2(t),\ldots x^{n-1}(t)\right), \qquad 1$$

describing systems with dissipation, where n represents order of the problem, or the special case,

$$\frac{d^n x}{dt^n}=f\left(t,x(t)\right), \qquad 2$$

for systems without dissipation. Generally, for an initial value problem (IVP), one seeks a solution, say $x(t)$, which satisfies n initial condition of the form

$$x^{(n)}(t_0)=x_0, \qquad 3$$

where $n=0,1,2,\ldots n-1$.

For the boundary value problems (BVP), the desired solution of (1) and (2) has to satisfy a boundary condition

$$r\left(x(a),x(b)\right)=0, \qquad 4$$

where $a\neq b$ are two different numbers and $r(u,v)=\begin{bmatrix} r_1(u_1,u_2,\ldots,u_n,v_1,v_2,\ldots,v_n) \\ r_n(u_1,u_2,\ldots,u_n,v_1,v_2,\ldots,v_n) \end{bmatrix}$ is a vector of n given functions r_i of $2n$ variables.

In what follows, the numerical approximation of solutions of IVP of ODE is discussed

2.1 Numerical Approximation of the Solutions of IVP of ODE

The numerical solution of mathematical models by ordinary differential equations, in particular initial value problems, has been widely studied. The most widely used numerical method for this class of problems is the finite difference methods. For BVP, any of the following methods can be employed: finite element methods and the semi-analytic methods such as homotopy perturbation method (He, 2008, 2009a; Jin, 2008; Liang and Jeffrey, 2009), the adomian decomposition method (Adomian, 1994), homotopy analysis methods (Kumar and Gupta, 2010; Liang and Jeffrey, 2009; Iiao, 1992; Yuen et. al., 2010; Zhu et. al., 2010), variational iterative method (He, 1999a, 2000; Nikkar, 2012), regular perturbation methods (Cole, 1968), etc. In the sequel, only finite difference methods for IVP of ODE shall be considered.

2.1.1 Finite Difference Methods

This is the most widely used numerical method to solve ordinary differential equations of the form (1), (or the special case (2), with either of the conditions (3) or (4). This method uses difference equations to approximate the solution of the problem. They include first order methods such as Euler's method, the family of Runge-Kutta methods, and higher order methods such as Runge-Kutta Nystrom method, the backward difference methods, and the continuous linear multistep methods (Lambert, 1973). The focus here shall be on the integration of the initial value problem (1) and (3) directly by continuous hybrid one step methods. For the purpose of this paper, second order problems, that is when $n=2$, which arise from the modeling in the domains of celestial and mechanical systems are considered (Hindamarsh, 1986).

Conventionally, to solve the initial value problem (1) and (3), one can either choose to reduce the problem to an equivalent system of first order equations and then use any of the first order methods or solve the problem directly using higher order methods. It has been reported in (Anake, 2012a, 2012b) however, that it is more convenient to solve the initial value problem (1) and (3) directly.

The continuous one step hybrid method uses the power series polynomial of the form

$$P(t)=\sum_{j=0}^{d} u_j t^j, \qquad 5$$

as the approximating polynomial on the partition $\pi_{[a,b]}: a=t_0<t_1<t_2<\cdots<t_{j-1}<t_j=b$ of the interval of integration $[a,b]$. The numerical scheme is developed by the combined techniques of interpolation and collocation. The approximating polynomial, expected to satisfy (1) and (3), takes the form

$$P(t)=\sum_{j=0}^{r+s-1} u_j t^j, \qquad 6$$

where r and s represent the number of interpolation and collocation points respectively. In particular, let us interpolate (5) at the origin and the fifth point, that is $r=2$ and collocate the differential system at nine points, that is $s=9$, in the one step hybrid design. It is worth mentioning, that this one step hybrid design incorporates

seven non-step points between the origin and the next step point. Thus, these eleven conditions imposed by the IVP (1) and (3) on (6) given as

$$P(t)=\sum_{j=0}^{10} u_j t^j = x_{n+r},\ r=0,5 \qquad 7$$

and

$$P'(t)=\sum_{j=0}^{10} j(j-1)u_j t^{(j-1)} = f_{n+s},\ s=0,1,2,..,8. \qquad 8$$

Leads to a system of eleven equations in eleven unknowns to be determined using any convenient method in the literatures.

By putting the unknowns obtained in the system (7) and (8) into (6), a one step numerical scheme is obtained in the form

$$x_{n+1}=\alpha_1(z)x_n+\alpha_2(z)x_{n+v_i}+h^2\left[\sum_{j=0}^{1}\beta_j(z)f_{n+j}+\sum_{i=0}^{7}\beta_{v_i}(z)f_{n+v_i}\right], \qquad 9$$

where, v_i indicates the non-step points, $h=t_{n+j}-t_{n+j-1}$ is a fixed step size, $t_{n+j}=t_n+jh$, $x_{n+j}=x(t_{n+j})$ approximates the exact solution at t_{n+j} and $f_{n+j}=f(t_{n+j},x_{n+j},x'_{n+j})$. The coefficients $\alpha_r(z)$ and $\beta_s(z)$ are obtained from the transformation of the unknowns obtained earlier using a scaling factor, $z=\frac{t-t_n}{h}$. For emphasis, note that (9) is completely determined by the coefficients $\{\alpha_r(z),\beta_s(z)\}$ for all values of $z\in[0,1]$.

Error issues concerning the scheme, (9) are considered by the concept of local truncation error. The local truncation error (*l.t.e*) is a simple concept that determines the difference between the approximate solution x_{n+j} and the exact solution $x(t_{n+j})$ when the step is taken with all earlier data exact. Typically, (9) satisfies *l.t.e* if

$$l.t.e=O(h^{p+2}) \text{ as } h\to 0,$$

where p, determined by relations among the schemes coefficients, is the order of accuracy of the scheme. Apart from analyzing error issues, for (9) to be valid, the nature of its convergence has to be established. To do this, it suffices to show that the method is consistent and zero stable according to (Henrici, 1962). Further more, the absolute stability of the scheme is investigated using either, boundary locus methods, Schurz criterion method or the Rout Hurwitz method (Lambert, 1973). This property guarantees that if the solution of the IVP (1) and (3) is bounded then, the numerical solution (9) is also bounded.

3. Models by Partial Differential Equations

Partial Differential Equations (PDE) are equations that involve rates of change with respect to two or more continuous variables. The distinction in the configuration of PDE problems unlike ODE problems makes it usually much harder to solve. However, simpler solutions exist for linear problems. Basically, PDE may arise from phenomena such as acoustics, fluid flow, electrodynamics, and heat transfer.

For a function F, the PDE is of the form

$$F\left(x_1,x_2,...,x_n,u,\frac{\partial u}{\partial x_1},...,\frac{\partial u}{\partial x_n},\frac{\partial^2 u}{\partial x_1\partial x_1},...,\frac{\partial^2 u}{\partial x_1\partial x_n},...\right)=0 \qquad 10$$

A solution of a PDE is generally not unique; additional conditions must generally be specified on the boundary of the region where the solution is defined. Basically, PDE are classified as parabolic, hyperbolic and elliptic. The classification provides a guide to appropriate initial and boundary conditions, and to smoothness of the solutions.

Several methods have been studied for the solution of PDE; this range from analytical through approximate analytical methods (He, 1998, 1999a, 1999b, 2000; Jin, 2006; Kumar and Gupta, 2010; Liang and Jeffrey, 2009; Liao, 1992; Nikkar, 2012; Yuen et. al., 2010; Zhu et. al., 2010) to numerical methods.

In this paper, only approximate analytical will be discussed.

3.1 Approximate Analytical Methods

By approximate analytical methods we refer to series expansion methods. These include the Adomian decomposition method (Adomian, 1994), the homotopy perturbation method (He, 1998, 1999a; Jin, 2006;Liang and Jeffrey, 2009), variational iteration methods (He,1999b, 2000; Nikkar, 2012), homotopy analysis methods (Kumar and Gupta, 2010; Liao, 1992; Yuen et. al., 2010; Zhu et. al., 2010), regular perturbation (Cole,1968), etc. They are especially suitable for non linear PDE. Note that, the Adomian decomposition method, the Lyapunov artificial small parameter method, and He's homotopy perturbation method are all special cases of the more general homotopy analysis method

(Liao, 1992). Except for the Lyapunov method, these methods are independent of small physical parameters as compared to the well known perturbation theory, which means greater flexibility and solution generality. In what follows, the Homotopy analysis method is discussed for the solution of nonlinear PDE arising from the mathematical modeling of physical phenomena.

3.1.1 The Homotopy Analysis Method (HAM)

The homotopy analysis method was first developed in 1992 by S. J. Liao, (Liao, 1992). The simple manner in which this method ensures the convergence of the solution series does not remove the fact that the method is a powerful mathematical tool for obtaining accurate enough approximations.

To describe the basic idea of HAM, consider the following nonlinear differential equation:

$$N\left[u(x,t)\right]=0, \qquad 11$$

where N is a nonlinear operator and the unknown function $u(x,t)$ is specified by the independent variables x and t. The zeroth-order deformation equation is derived by means of HAM as follows:

$$(1-p)L\left[\phi(x,t;p)-u_0(x,t)\right]=\hbar H(x,t)N\left[\phi(x,t;p)\right], \qquad 12$$

where $p\in[0,1]$ is the embedding parameter, $\hbar\neq 0$, is a nonzero auxiliary parameter, $H(x,t)\neq 0$, is an auxiliary function, L is an auxiliary linear operator, $u_0(x,t)$ is the initial guess of $u(x,t)$. We can see that when the embedding parameter changes from $p=0$ to $p=1$, the function $\phi(x,t;p)$ varies from the initial guess $u_0(x,t)$ to the exact solution $u(x,t)$. Now, expanding $\phi(x,t;p)$ in Taylor series with respect to p gives

$$\phi(x,t;p)=u_0(x,t)+\sum_{k=1}^{\infty}p^k u_k(x,t), \qquad 13$$

where

$$u_k(x,t)=\frac{1}{k!}\frac{\partial^k\phi}{\partial p^k}\bigg|_{p=0} \qquad 14$$

The parameter $\hbar$ controls the convergence of the series (13) such that if it is convergent at $p=1$, we have

$$\phi(x,t;p)=u_0(x,t)+\sum_{k=1}^{\infty}u_k(x,t).$$

As proven earlier in [19], this must be one of the solutions of (11).

Substituting (13) into (11) and equating the coefficients of like powers of p, the m^{th}-order deformation equation is obtained as follows:

$$L\left[u_m(x,t)-\chi_m u_{m-1}(x,t)\right]=\hbar R_m\left(\overline{u}_{m-1}(x,t)\right), \qquad 15$$

subject to the initial conditions

$$u_i(x,0)=0 \qquad 16$$

where the vector $\overline{u}_n(x,t)=\{u_0(x,t),u_1(x,t),\ldots,u_n(x,t)\}$.

$$R_m\left(\overline{u}_{m-1}(x,t)\right)=\frac{1}{(m-1)!}\frac{\partial^{m-1}N\left[\phi(x,t;p)\right]}{\partial p^{m-1}}\bigg|_{p=0}$$

and

$$\chi_m=\begin{cases}0, & m\leq 1,\\ 1, & m>1.\end{cases}$$

Thus, the solution of the m^{th}-order deformation equation (15) for $m\geq 1$ becomes

$$u_m(x,t)=\chi_m u_{m-1}(x,t)+\hbar\int_1^t R_m\left(u_{m-1}(x,\tau)\right)d\tau+c, \qquad 17$$

where c is the integration constant determined by the initial condition (16). This way, we obtain the solution of (11) as

$$u(x,t)=\lim_{N\to\infty}\Phi_N(x,t) \qquad 18$$

where

$$\Phi_N(x,t)=\sum_{m=0}^{N-1}u_m(x,t).$$

The main advantage of the HAM is that it always provides one with a simple way to adjust and control the convergence radius of solution series (Liao, 1992). Different from perturbation techniques, the HAM is valid no matter if a nonlinear problem contains small/large physical parameters; be it a strongly nonlinear system or a weakly nonlinear cases.

4. Simulations

It is a well known fact that even though mathematical equations can be formulated to model systems, these equations are many times analytically intractable. In these situations, a computer can implement the mathematics literally and repeatedly to very extreme advantages. Both methods discussed above for instance, lend themselves easily to computer simulations. Infact, the implementation of the scheme (9) is only realistic when a computer program is written to simulate the result at the respective grid points. Similarly, symbolic computation programs such as maple, mathematica or matlab are employed to obtain the solutions in (17).

5. Conclusion

The role of mathematical models and simulation in the development of clean technology is revealed in the methods discussed for the solutions of ordinary and partial differential equations. Systems and phenomena that lead to IVP of ordinary differential equations and nonlinear partial differential equations are clearly understood and can be interpreted from the solutions of these mathematical models. In this paper, one method each for the solutions of models by ODE and models by PDE respectively has been discussed. These methods are by no means the only methods available as earlier mentioned, but they seemed the most convenient for this discussion.

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