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Mathematical modeling of carbon nano structures using symbolic computing

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Abstract*—A mathematical model is a description of a system using mathematical concepts and language. The process of developing a mathematical model is termed as mathematical modeling. Symbolic computation is study and development of algorithms and software for manipulating mathematical expressions. Computer algebra system is software program that facilitates symbolic mathematics. There are many commercial Computer algebra system softwares like Mathematical, Matlab, Maple and Non Commercial softwares like Maxima, GiNaC, SymPy, Sage, Axiom are available. This Paper is about Mathematical modeling of carbon nano structures for CSIR-4PI Lab using symbolic computation by using Sage-Maxima. Here goal is Mathematical modeling by using free software instead of Mathematical. Differential transformation method is used to solve differential equations in mathematical modeling.

***Index Terms*—Symbolic Computing, Sage, Maxima, Carbon nano structures, Mathematical modeling, SymPy, Mathematical, Differential transformation**

I. INTRODUCTION

Nanotechnology has attracted many researchers and become popular after the invention of carbon nanotube. The mechanical, electrical and thermal properties of carbon nanotubes are superior as compared to any other materials. The mechanical analysis of carbon nanotubes can be performed by experimental, atomic simulation and continuum modeling. Experimental setup is difficult because controlling the parameter at nanoscale is a tough task. The atomic simulation involves atom level to macro level computing and it leads to high cost of analysis and high performance computing. The continuum modeling is efficient and can be performed with less computing and understanding the physical behavior in a reliable manner. After working with different CAS softwares GiNaC, SymPy, Sage, maxima selected maxima because of its arbitrary-precision arithmetic, which is needed in Differential transformation method. Sage is having interface to maxima and it can function as an integrator of other diverse computer algebra systems. Selected Sage and for programming. Here is a brief overview of Computer Algebra Systems.

A. Maple

Developed and sold by Waterloo Maple Inc. (Maple soft), the Maple mathematics software package was first created in 1981 by the Symbolic Computation Group at the University of Waterloo in Waterloo, Ontario, Canada. Maple is an impressive-looking package that is especially adept at three-dimensional graphing and at displaying mathematical formulae in textbook form. It combines an interface and a programming language into a dynamic tool for both numerical and symbolic problem solving. Many universities have standardized on Maple for teaching mathematical concepts. The company offers student and professional versions of the software.

B. Mathematica

Stephen Wolfram's company, Wolfram Research, developed Mathematica in the late 1980s with a heavy emphasis on the programming aspects of the tool. It offers a flexible combination of both procedural and functional programming and introduces a non deterministic method for the automatic rewriting of formulae. It's a powerful software package with a large and diverse library of functionality, and it offers a unique multiple-paradigm way for solving problems.

Free softwares

A. GiNaC

GiNaC, unlike most other computer algebra systems, doesn't provide a graphical user interface (GUI) for the input of expressions, preferring that the user input expressions in native C++ (the implementation language). It accomplishes algebraic syntax by using the native C++ object-oriented technique of operator overloading.

B. Maxima

Like most computer algebra systems, Maxima is written in Lisp. Based on the commercial package Macsyma, Maxima includes a complete ALGOL-like programming language and is most useful for teaching programming concepts in computer algebra. It offers arbitrary-precision arithmetic so that integers and rational numbers are limited in size only by the system's available memory.

C. Sage

Software for Algebra and Geometry Experimentation (SAGE) is written in Python and uses the interactive Python shell as its user interface. SAGE is unique in that it can function as an integrator of other diverse computer algebra systems, allowing the user to leverage the individual strength of various packages.

D. SymPy

SymPy is a Python library for symbolic mathematics. It aims to become a full featured computer algebra system (CAS) while keeping the code as simple as possible in order to be comprehensible and easily extensible. SymPy is written entirely in Python and does not require any external libraries.

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Differential Transformation method

The differential transformation technique converts the governing differential equation into an algebraic recursive equation, which must be solved together with the differential transformation of the boundary conditions. Although a fairly large number of terms are required for convergence of the solution, the differential transformation method is nonetheless efficient and fairly easy to implement. The method is also shown to be very accurate when compared with a known analytical solution.

II. AXIAL VIBRATION ANALYSIS OF NANO RODS WITH NONLOCAL CONTINUUM ELASTIC THEORY

Axial vibration of nano rods are analyzed using nonlocal continuum elastic model. The governing equation for the free-vibrating axial rod with nonlocal elasticity is defined as[3]

$$EA\partial^2 u/\partial x^2 = (1-(e_0 a)^2\partial^2/\partial x^2)m\partial^2 u(x,t)/\partial t^2 \quad (1)$$

Here A, E are the area & Young's Modulus of the nano rod, u is axial displacement, m is mass per unit length, 'a' is the internal characteristic length and e_0 is a constant. The value of $e_0 a$ is crucial to ensure the validity of nonlocal models. When the absence of nonlocal parameters $e_0 a$ = 0, the classic rod model results are obtained. The solution of equation (1) is assumed as harmonic vibrations and using the method variable separation

$$u(x,t) = u(x)e^{i\omega t} \quad (2)$$

Substitute the Equation (2) in Equation (1) and following differential equation obtained

$$d^2u/dx^2 + \beta^2 u = 0 \quad (3)$$

Where

$$\beta^2 = \Omega^2/1-(e_0 a/L)^2\Omega^2,$$

$$\Omega^2 = m\omega^2 L^2/EA \quad (4)$$

Where Equation (4) represents dimensionless frequency.

Apply DTM, and the Equation (3) becomes

$$U(k+2) = -\beta^2 U(k)/(k+1)(k+2) \quad (5)$$

Clamped Clamped Boundary Condition

u(0) = u(L) = 0 (6)

Clamped Free Boundary Condition

u(0) = N(L) = 0 (7)

The boundary conditions from Equation (6) and (7) are also transformed using DTM Clamped Clamped Boundary Condition using DTM

U(0) = 0, U(1) = c1 (8)

$$\sum_{k=0}^{\infty} U(k) = 0 \quad (9)$$

Clamped Free Boundary Condition using DTM

U(0) = c1, U(1) = 0 (10)

$$\sum_{k=0}^{\infty} U(k) = 0 \quad (11)$$

The Equation (9) and (11) are solved for the appropriate boundary conditions by using recurrence relation of Equation (5) for the non trivial solution of value β^2 using Maxima and compared results with Matlab. Here four decimal precision is considered for the convergence of the value of β^2 and k = 50 terms are required for convergence of first five values of β^2. The results are shown in Table 1. From the Equation (4), the effect of nonlocal parameter over frequency can be analyzed using $e_0 a$= 0 to 0.1 In this study Maxima results are compared with Matlab and very good close matching is observed as shown in Table 1. First five values are shown in Table 1.

Table 1. First five values of β^2 of nanorod

Boundary Condition	Maxima	Matlab
Clamped Clamped	9.8696	9.8696
	39.4784	39.4784
	88.8264	88.8264
	157.9136	157.9136
	246.7401	246.7401
Clamped Free	2.4674	2.4674
	22.2066	22.2066
	61.6850	61.6850
	120.9026	120.9026
	199.8594	199.8594

III. VIBRATION OF CARBON NANOTUBE

The nonlocal Timoshenko vibration of carbon nano tube model without nonlocal effect of shear stress obtained from Wang [1] has been modified to account for winkler and Pasternak elastic medium [2] can be written as [4]

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$$\beta AG(\partial\Psi/\partial x + \partial^2 W/\partial x^2) + (e_0 a)^2(k_W \partial^2 W/\partial x^2 - k_G \partial^4 W/\partial x^4$$

$$+\rho A\partial^4 W/\partial x^2 \partial t^2 = k_W W - k_G \partial^2 W/\partial x^2 + \rho A\partial^2 W/\partial t^2$$

(12)

$$EI\partial^2\Psi/\partial x^2 - \beta AG(\Psi + \partial W/\partial x) = \rho I\partial^2\Psi/\partial t^2 - (e_0 a)^2 \rho I\partial^4\Psi/\partial x^2\partial t^2$$

(13)

Here I is moment of inertia, G shear modulus, ρ Mass Density, β is shear coefficient factor. W(x , t) is transverse displacement. Ψ(x , t) is rotation of the cross section. k_W Winkler modulus. k_G Shear modulus of the elastic medium. After converting to a system of Ordinary Differential Equations, Need to apply Differential transformation method.

Assume k_W = 0 and k_G = 0.Equations will become [4]

$$W(K+2) = -\Psi(k+1)/i + 2 - aS^2 W(K)/(i+1)(i+2)$$

(14)

$$\Psi(k+2) = (1 - aS^2 r^2)\Psi(k)/S^2(i+1)(i+2) + W(i+1)/S^2(i+2)$$

(15)

where

$S^2 = EI/\beta AGL^2$,

$r^2 = I/AL^2$

(16)

The Equation (14) and (15) are solved with appropriate boundary conditions for 'a' using Maxima and compared results with Mathematica. Here four decimal precision is considered for the convergence of the value of 'a' and k = 50 terms are required for convergence of first four values of 'a'. The results are shown in Table 2.

Table 2. First four values of 'a'

Boundary Condition	Maxima
Simply Supported	3.0915
	5.9317
	8.4242
	10.5917
Clamped Clamped	4.4423
	6.9338
	9.1304
	11.0666
Clamped Free	1.8606
	4.4677
	7.0912
	9.3517
Clamped Simply Supported	3.7809
	6.4595
	8.7948
	10.8395

IV. CONCLUSION

Axial vibration of nano rods is analyzed using Maxima and compared results with Matlab and The nonlocal Timoshenko vibration of carbon nano tube is analyzed. The values of β^2 and 'a' are converging very good by using maxima.

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