3

COMPUTATIONAL MECHANICS

We have continued our work on development and application of novel Homotopy Analysis Methods. We have demonstrated the advantage of using the modification of the Homotopy Analysis Method with a non homogeneous term for a system of equations for the first time. We have also developed a Homotopy Analysis Method with an optimal distribution of the initial conditions in a shooting method to solve two point boundary value problems.

Computational nanomechanics focuses on nonlocal continuum modelling and molecular dynamics simulations in nanomaterials. Parallel Super Computers are used to analyse and simulate the properties of new materials (nanomaterials) from the nano to macroscale. This reduces the cost of expensive experimental analysis. Studies have been carried out on a nonlocal continuum theory for modeling the buckling of Carbon Nanotubes. We have calibrated the nonlocal small scale parameter from Molecular Dynamics simulations and we have shown that the approach currently used in the literature may lead to inaccurate results. We have demonstrated the efficiency of some open source software for solving these problems.

Inside

3.1 Influence of Thermal Radiation on Unsteady Flow over a Contracting Cylinder with Thermal-Diffusion and Diffusion-Thermo Effects by HAM with Non-Homogeneous Term

An analytical study is carried out to present the thermal radiation, Dufour and Soret effects on unsteady viscous flow over a contracting cylinder. The coupled nonlinear partial differential equations are transformed into a system of coupled nonlinear ordinary differential equations by using a suitable similarity transformation. The homotopy analysis method (HAM) and HAM with a non-homogeneous term are employed to obtain analytical solutions for the system of coupled nonlinear ordinary differential equations through the minimization of the averaged square residual error. The inclusion of the non-homogeneous term is presented to further minimize the average square residual error (Δ). We observe a better convergence in comparison to HAM solutions. To the best of our knowledge this is the first application to a system of coupled nonlinear differential equations where the idea of the inclusion of the non-homogeneous term is used. We present the convergence analysis for the solutions obtained by HAM and HAM with a non-homogeneous technique in Tables [3.1] and [3.2]. It is clear from these tables that with the latter approach HAM with a non-homogeneous term gives better convergence and minimum square residual error in comparison to standard HAM approach.

Table 3.1 The averaged square residual error with varying at 10th order of approximation with standard HAM (without non-homogeneous term) technique $\Pr = 1, S = -1, Sc = 0.65, Sr = 1,$ $Du = 0.06,\ R_d = 10.$

h	Δ
-0.25	0.002751320
-0.26	0.002231060
-0.27	0.001805630
-0.28	0.001459880
-0.29	0.001184700
-0.30	0.000982196
-0.31	0.000879418
-0.32	0.000963043
-0.33	0.001463140
-0.34	0.002952130
-0.35	0.006827180

Table 3.2 The averaged square residual error with varying at 10th order of approximation with non-homogeneous term $\mathrm{F}(\eta) = \mathrm{c}_1 \mathrm{e}^{-\eta}$ and for optimal $\mathrm{h} = -0.31,\quad \Pr = 1, S = -1, Sc = 0.65, Sr = 1,$ $Du = 0.06,\ R_d = 10.$

c_1	Δ
0.5	0.000716046
0.6	0.000694628
0.7	0.000676962
0.8	0.000663048
0.9	0.000652887
1.0	0.000646477
1.1	0.000643820
1.2	0.000644914
1.3	0.000649761
1.4	0.000658360
1.5	0.000670711

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3.2 Homotopy Solutions for Nonlinear Problems with Two-Point Neumann Boundary Conditions

We study a comparison of modified versions of Rational Homotopy Perturbation Method (RHPM) and homotopy analysis method (HAM) to solve two-point nonlinear problems with Neumann boundary conditions which very often arises in physical systems. The modification of RHPM relies on the strategic distribution of the Neumann boundary conditions among the different iterations. RHPM gives solutions assuming the form of solution to be a rational polynomial and then using the distribution of boundary conditions throughout the different orders. HAM coupled with a shooting technique gives good results in a very simple and straightforward way with fewer assumptions. The results of both methods are accurate with respect to the exact solution of the problems considered. Nonetheless, RHPM requires only a second order approximation to obtain similar results in comparison to the seventh order HAM approximation. To check the efficiency of the proposed modifications we solve two nonlinear problems with given Neumann boundary conditions one is Bratu's problem and other is Burger's equation. The comparative results for the Bratu's and the Burger's equation are shown in Table [3.3] and [3.4].

Table 3.3 The comparative study for the solution of Bratu's problem with the proposed second order RHPM and the proposed seventh order HAM with the exact solution.

X	RHPM solution	HAM solution	Exact solution
0	0	0	0
0.1	0.00987156	0.0100167	0.0100167
0.2	0.04000446	0.040271	0.040270
0.3	0.09119138	0.0914016	0.091383
0.4	0.16446022	0.164556	0.164458
0.5	0.26133364	0.261514	0.261168
0.6	0.38410832	0.384852	0.383930
0.7	0.53620148	0.538116	0.536172
0.8	0.72263494	0.725982	0.722781
0.9	0.95077066	0.954324	0.950885
1.0	1.23125000	1.230100	1.231250

Table 3.4 The comparative study for the solution of Burger's problem with the proposed second order RHPM and the proposed seventh order HAM up to fifth terms of sin (2x) with the exact solution.

x	RHPM solution	HAM solution	Exact solution
0	0	0	0
0.1	0.09988958	0.0998334	0.0998334
0.2	0.19879931	0.198668	0.198669
0.3	0.29566654	0.295511	0.295520
0.4	0.38951433	0.389379	0.389418
0.5	0.47943371	0.479311	0.479426
0.6	0.56456849	0.564369	0.564642
0.7	0.64410435	0.64366	0.644218
0.8	0.7172632	0.716345	0.717356
0.9	0.78330427	0.781668	0.783327
1.1	0.89131935	0.887798	0.891207
1.2	0.93212389	0.927808	0.932039
1.3	0.96353598	0.958955	0.963558
1.4	0.98531969	0.981452	0.98545
1.5	0.99746956	0.995789	0.997495
$\pi/2$	1.00039043	1.00138	1.000000

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3.3 Small Scale Parameter Calibration for Buckling Analysis of Carbon Nanotube using Molecular Dynamic Simulation

The aim of the present study is to improve nonlocal continuum elasticity theory for Carbon Nanotubes (CNT) by calibrating its small scale parameter. In this work, the small scale parameter of the Nonlocal Timoshenko beam model and the Nonlocal shell model has been calibrated. Despite the high number of studies conducted on the buckling of CNTs, there are still several issues that are not addressed sufficiently like change of properties with chirality and aspect ratio of CNTs since most of the studies conducted on buckling of CNT are based on continuum mechanics which is used conveniently to analyze large-scale problems. However continuum theory cannot address small size effect problems. Hence to overcome this drawback, nonlocal continuum theory was developed.

Nonlocal continuum theory uses a small scaling parameter (e_o) to address this nanoscale problem and can also be used to address the chirality effect of CNTs but some arbitrary value is taken on the basis of trial and error and leads to inaccurate results. In this work Molecular Dynamics Simulation (MDS) is used to calibrate this small scale parameter value and an empirical relation has been developed which can be directly be used in the nonlocal continuum theory to study the mechanical properties of CNT.

In this work Molecular Dynamic Simulation (MDS) has been used to calculate the critical buckling load and the critical buckling strain. The Figure 3.1 shows compressive load vs strain diagram for a (16, 0) zigzag Carbon Nanotube with 1.25 nm diameter and 10 nm length.

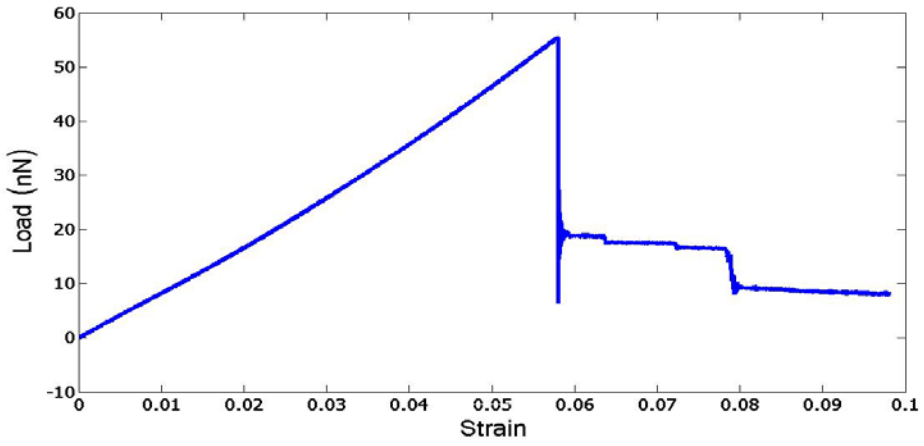

Figure 3.1 Critical buckling load vs Critical Strain

As is seen in the Figure 3.1, the load increases with strain but at a point it fails and there is a sudden drop in load, the strain at this point where it loses its load carrying capacity is called its critical strain and maximum load at this point is called Critical Buckling load. The Carbon Nanotube under goes two modes of buckling, namely column and shell buckling. Critical Buckling load analysis has been carried out for CNT for various diameters ranging from 0.5 nm

to 2 nm for various chiral angles of the Carbon Nanotube (0°, 5° & 30°). It is found that the buckling mode depends on its diameter. A transition diameter is 1nm. Carbon nanotubes below 1nm show column buckling and above 1nm show shell buckling which is also shown in Figures 3.2 and 3.3.

In the shell buckling diagram a (16,0) a zigzag Carbon Nanotube, with a diameter of 1.25 nm shows shell buckling at strain of 0.05783 whereas the (7,7) Carbon Nanotube where the diameter is 0.949 shows column buckling at strain of 0.04305.

Figure 3.2 Column Buckling of (7,7) Carbon Nanotube

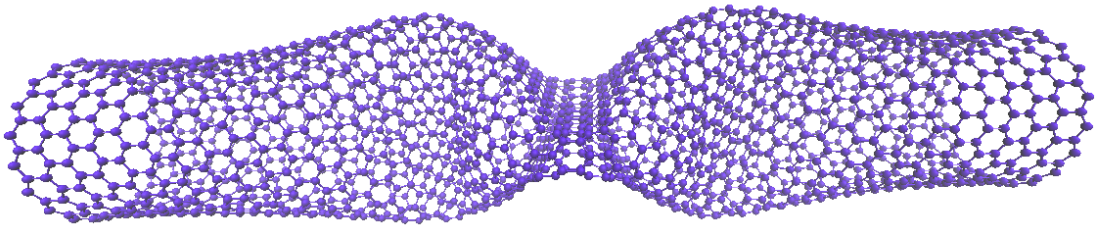

Figure 3.3 Shell Buckling of (16,0) Carbon Nanotube

From this Molecular Dynamic Simulation Study Critical data, it is shown that a single fixed small scaling parameter cannot be used in every condition (chirality and aspect ratio) as it will yield inaccurate results. This MDS data is used to generate the small scaling parameter data for nonlocal continuum theory for nonlocal the Timoshenko Beam model and the Nonlocal Shell model and small scaling parameter data is used to develop empirical relations for nonlocal continuum theory which can be directly used in without selecting any particular small scaling parameter value.

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3.4 Symbolic Computation Analysis of One-Dimensional Nanostructures using Open Source Software

There are many commercial computer algebra system software like Mathematica, Matlab, and Maple which are available at high cost. Many non commercial software like Maxima, GiNaC, SymPy, Sage, Axiom are available as open source packages. Here, the structural behaviour of

carbon nanostructures are investigated using symbolic computation with open source software Sage-Maxima. This symbolic computing packages gives quick solutions compared with numerical analysis. For larger computations, parallel computation is required to study the mathematical model.

Mathematical models of carbon nanorods and nanotubes are studied by using the open source computer algebra system (CAS) software Maxima. Vibration analysis of nanorods and buckling behaviour of carbon nanotubes are carried out using continuum elasticity modeling. It has been observed that the open source software Maxima is comparable with proprietary software in giving reliable results and the execution time is very small for linear problems. It is difficult to simplify and solve more complex equations by using Maxima. SymPy can be used to solve complex equations but the excecution time has to be compromised with the simple implementation methodology. This can be achieved through the Super Computer facility available in the institute. SAGE and SymPy have been installed in the Super Computer "Cluster Platform 3000 BL460c with 1084 nodes Gen8". It can be used to solve complex equations and higher order polynomials (order > 200) using SAGE parallel programming.

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