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COMPUTATIONAL MECHANICS

Sophisticated mathematical modelling aided by powerful computing and visualization has the potential to provide the cutting-edge to industry; generation of cost-effective solutions, process optimization and product design are some of the areas where modelling and simulation can play critical to enabling role. The C-MMACS Computational Industrial Mechanics Programme (CIMP) seeks to develop and apply tools of mathematical modelling and computer simulation in diverse areas of engineering.

INSIDE

3.1 The Dynamics and Rheology of Periodically Forced Spherical Particles in a Quiescent Newtonian Fluid at Low Reynolds Numbers

The effects of both convective and unsteady inertia have been studied on the dynamics and rheology of a dilute suspension of periodically forced neutrally buoyant spherical particles, at low Reynolds numbers, in a quiescent Newtonian fluid. The inclusion of inertia results in additional terms in the equation governing the dynamics of the particle that represent a fading memory for the entire history of the motion. The inclusion of convective inertia in the low Reynolds number limit makes the memory term nonlinear. Several tests were performed to show that the numerical results for this problem are physically reasonable and correct. A perturbation analysis of the problem yields strong evidence for the results of our simulations being correct. It is observed that there is a preferred direction in this system which manifests itself in the properties of the solution. This preferred direction is identified as the direction of the initial motion of the particle. We present here, results of the behavior of various parameters with respect to Reynolds numbers and the amplitude of the periodic force. These include phase space plots between particle displacement and particle velocity and the variation of a rheological parameter, namely the normal stress with respect to Reynolds number and the amplitude of the periodic force. We feel that our results may be technologically important since the rheological parameter depends strongly on controllable parameters such as the Reynolds number and the amplitude of the periodic force. Further this system is one of the simplest systems whose rheology shows non-Newtonian behavior, such as the presence of a normal stress.

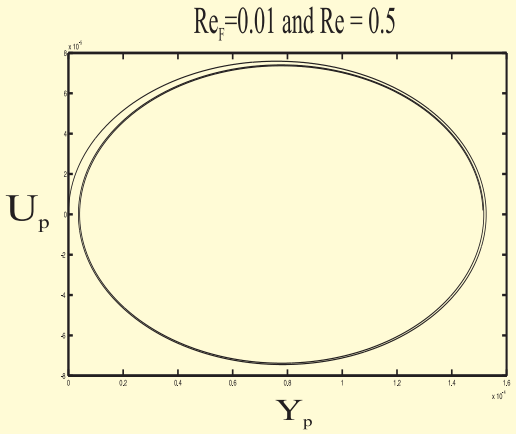

Figure 3.1 The phase space attractor for ReF = 0.01 and Re = 0.5, the earlier result had kinks and discontinuities in this region.

In the current year we improved our simulation at low amplitudes of the periodic forcing, near the region ReF ~ 0.01. We reduced the error term in the upper limit of the integral term of the governing equation and have eliminated the discontinuities and kinks in the numerical solutions in these regions. The drawback of this was that the numerical simulation consumed a lot of computational time to generate the solution (almost 2 months on the SGI Altix 350 machine).

T R Ramamohan, K Madhukar and I S Shivakumara

3.2 Dynamic Analysis of Double-Walled Carbon Nanotube

The present study deals with determination of the natural frequencies of a double walled carbon nanotube under various boundary conditions. A simple and powerful semi-analytical method is used for the evaluation of the frequencies using symbolic computations. Four different boundary conditions are used such as clamped-clamped, clamped-free, simply supported and clamped-hinged. The present approach is compared with Analytical, Bubnov-Galerkin and Petrov-Galerkin methods available from literature. Though the approximated solutions are comparable within error percentage, the present frequency results are more accurate, easy implementation, and quick and effective determination of frequencies. It is observed that the inner tube frequencies are small compared to higher magnitude of outer tube frequencies. The effect of slenderness ratio length to diameter study shows that the frequencies of inner and outer tube are decreasing with increasing slenderness ratio. Table 3.1 shows that the present semi-analytical method determines identical results compared to exact solutions for the case of simply supported boundary conditions. As the slenderness ratio (L/d) increase, the fundamental frequency decreases. There is no analytical solution for the simply supported and clamped boundary effect over the frequencies. However the present approach yields better results compared to other methods. The Bubnov-Galerkin and Petrov-Galerkin method gave the approximate range of the solution. The present method can be used as an alternative for the analytical solution because of its accuracy with any boundary conditions.

Table 3.1 Fundamental frequencies for double-walled carbon nanotube with simply supported condition

L/d	10	11	12	13	14	15	16	17	18	19	20
Present	0.46830	0.38707	0.32527	0.27716	0.23899	0.20819	0.18298	0.16209	0.14458	0.12976	0.11711
Exact	0.46830	0.38707	0.32527	0.27716	0.23899	0.20819	0.18298	0.16209	0.14458	0.12976	0.11711
Bubnov	0.47211	0.39021	0.32791	0.27942	0.24093	0.20988	0.18447	0.16341	0.14576	0.13082	0.11806
Duncan	0.46863	0.38734	0.32550	0.27736	0.23916	0.20834	0.18311	0.16221	0.14468	0.12986	0.11720
Petrov	0.46884	0.38751	0.32564	0.27748	0.23926	0.20843	0.18319	0.16228	0.14475	0.12991	0.11725

V Senthilkumar

3.3 Axial Vibration Analysis of Nanorods using Nonlocal Continuum Model

Nanotechnology is popular among the researchers due to the fact that small sized carbon nanotubes have high mechanical strength. Molecular dynamics simulation is expensive and difficult for large scale systems. Hence continuum models are used to study the behavior of nanostructures. In the present study, the axial vibrations of nanorods are analyzed using nonlocal continuum elastic models. The present work deals with the study of small scale effect on vibration frequencies of nanorods. The use of simple semi-analytical methods calculates the vibration frequencies of nanorods. Two different boundary conditions like clamped-clamped (CC) and clamped-free (CF) are used to study the nonlocal effects of nanorods.

Table 3.2 First five values of frequency of nanorod for CC and CF boundary conditions

Boundary Condition	Present	Exact
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

The validity of nonlocal models is determined by matching the dispersion curves based on the atomic models. When the absence of nonlocal parameters e0a = 0, the classic rod model results are obtained. In the present approach, a semi-analytical numerical method called differential transform method (DTM) is used for the nanorod vibration analysis. DTM was successfully applied for nonlocal beam models and proved its capability of analyzing nanotubes. Continuum models are solved for the appropriate boundary conditions by using the recurrence relation for the non-trivial solution using symbolic tools of MATLAB. Here four decimal points precision is considered for the convergence of the frequency value. The results are shown in Table 3.2. It has been observed that the effect of nonlocal parameter over frequency ω can be analyzed using e0a = 0 to 0.1 values and it is very clear that nonlocal parameter has affected the frequency when the nonlocal model is considered. The present results are compared with analytical solutions and a very good close agreement is observed between the analytical and the present semi-analytical method.

V Senthilkumar

3.4 Vibration Analysis of Single Walled Carbon Nanotube

Invention of carbon nanotubes heralded a new era in nanotechnology research. Because of their high mechanical strength, electrical and thermal conductivity, carbon nanotubes are superior to other materials. The classical continuum model has not account for nonlocal effects for the structural behavior of nanotubes. So the nonlocal continuum theory was proposed by Eringen for the analysis of nanotubes as an alternative method for molecular dynamics simulations because of its easy analysis of implementation and little computational effort. The nonlocal Timoshenko beam models are used to analyze the vibration behavior of carbon nanotubes with shear deformation effects. The dynamic behavior of a single-walled carbon nanotube has been studied with nonlocal continuum elasticity models using a differential transform method. By using a Differential Transformation Method (DTM), the closed form series solution or an approximate solution can be obtained for the differential equation. The small scale effect on vibration frequency has been examined for the effects of transverse shear deformation using a nonlocal Timoshenko model.

Table: 3.3 Timoshenko Frequency for Simply Supported SWCNT for various nonlocal parameters

	0		0.1		0.3		0.5		1.0	
L/d	Exact	Present	Exact	Present	Exact	Present	Exact	Present	Exact	Present
10	3.0929	3.0916	3.0243	3.0231	2.6538	2.6531	2.2867	2.2863	2.0106	2.0103

The nonlocal Timoshenko frequencies of the SWCNTs have been computed from the recursive relation and the associated boundary conditions. A MATLAB computer code has been developed to implement the differential transfer procedure technique and the vibration frequency (Ω) has been computed. In the computation of Ω values of the SWCNT Young's modulus, E=5.5 TPa, shear correction factor Ks = 0.563 and nanotube diameter as 0.678 nm are considered. Sensitivity of these results to the number of terms employed in the DTM is investigated. The convergence of the solutions of Ω with various number of terms used in DTM for simply supported (SS), clamped - clamped (CC), clamped - simply supported (CS) and clamped - free (CF) boundary conditions are investigated. These results are compared with corresponding exact solutions available in literature. It can be observed that the exact solutions and the present DTM solutions are in very good agreement. From the Table 3.3, it has been observed that the nonlocal parameter has influenced the Timoshenko frequency for the case of a Simply Supported SWCNT.

V Senthilkumar, S C Pradhan and G Prathap

3.5 Rheology and Dynamics of Periodically Forced Suspension at Finite Reynolds Number

The rheological properties of suspensions are important in design and in processes in many industries (e.g., suspension coating and slurry transport, chemical process industries), biological processes and in nature. At the early stage of investigation most attention was paid to understand viscous suspensions at low particle Reynolds numbers and at dilute particle concentration. Under dilute conditions, hydrodynamic interactions between particles can be neglected and the suspension exhibits Newtonian rheology. Deviations from Newtonian behavior are observed at higher solid volume fractions.

Different classes of macroscopic behaviour of particulate suspensions have been reviewed under some generalized categories such as steady state behaviour, periodic behaviour, quasi-periodic behaviour, and chaotic or stochastic behaviour that have either been observed experimentally or predicted through simulation. A comprehensive study has also been carried out on correlations between micro-dynamical properties and the macroscopic rheological behaviour of the suspension. We highlight the effects of an external field, either a periodic force or periodic shear and the effect of hydrodynamic interactions in the case of semi dilute suspensions on rheological behaviour. In consideration of studying the effect of an external periodic field on the macroscopic rheological behaviour of the suspension at higher Reynolds number, we have critically reviewed different aspects of one promising computational fluid dynamics technique, which we plan to use in our future work namely the lattice-Boltzmann

method (LBM). Different states of particulate suspensions such as jamming, shear thinning, and shear thickening where macroscopic rheological properties are functions of time but the function of experimentally controlled parameters such as a constant shear rate have also been summarized.

Our previous research on periodically forced particulate suspensions at zero Reynolds number predicts that chaotic dynamics at the micro level shows chaotic rheological behaviour at macro level. To the best of our knowledge this has been observed for the first time in the world. Here we extend our previous research to finite Reynolds number. Such a study will yield insights on the relationship between individual particle dynamics and collective macroscopic dynamics and explore the possibility of developing technologically important smart fluids. The state of the art is as follows. At first we have considered that the fluid drag acts as a point force on the particle of finite size and 2D Lattice-Boltzmann method has been developed for simulating the fluid phase and molecular dynamics (Newtonian mechanics) type modeling has been implemented and coupled with the LBM to track the individual particle in a Lagrangian manner. To handle particle-particle collisions we have implemented the collision algorithm using a link-list algorithm. The fluid phase LBM code has been validated by running simulations for Couette and Poiseuille flow as shown in Fig. 1. The next stage is to implement the LBM code for studying fully resolved fluid-particle suspensions.

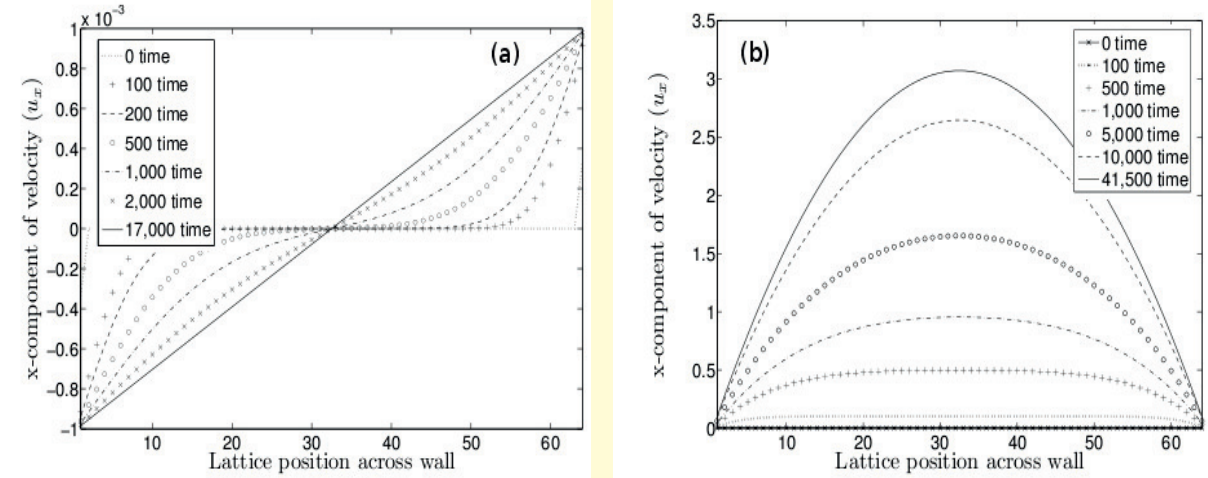

Figure 3.2 Velocity evolution of the fluid phase with time for (a) Couette flow and (b) Poiseuille flow

A new initiative is being taken up to develop software modules using the Lattice Boltzmann Method (LBM) to study the behaviour of complex-fluids such as fluid-particle suspensions, flow through deformable surfaces etc. Besides studying the dynamics and rheology of periodically forced suspensions at finite Reynolds numbers issues related to fluid-structure interaction (FSI) which occur in fluid flow through deformable surfaces will also be investigated by coupling the LBM and finite element model (FEM). The long term objective is to develop multipurpose software based on Lattice Boltzmann methods for solving fluid flow and heat transfer problems in engineering and bio-fluidics applications.

Partha S Goswami and T R Ramamohan

3.6 Homotopy Analysis Method Including Non Homogeneous Auxiliary Linear Operator

The Homotopy analysis method does not require the existence of a small parameter, which is required for perturbation techniques, and thus is valid for both weakly and strongly nonlinear problems. It is difficult to determine analytical solutions to nonlinear equations, except in some cases. Finding analytical solutions by homotopy analysis method is a popular choice because implementation of this technique is relatively easy. The convergence of the solution series found by any method is a primary requirement. In this method we can adjust and control the convergence of solution series by a convergence control parameter h, present in the frame work of HAM. For difficult problems there is a need to go to higher orders to get more accurate solutions. This involves great time and computational cost. To reduce the computational cost and time, we have included a non-homogeneous term in the auxiliary linear operator, so-that we obtain the same or a more accurate solution in a fewer number of iterations.

To show the efficiency of this technique we present an analysis of the following problem. We also prove a convergence theorem.

Consider the following non-linear differential equation:

$$V'(t)+V^2(t)=1, \quad V(0)=0, t\geq 0$$

The exact solution of the equation is $tanh(t)$.
The above equation is solved by using non-homogeneous auxiliary linear operator and compared with Liao's (2003) solution.

The solutions obtained for different order of HAM approximations using both the schemes are presented in the following table and corresponding h-curves are shown in Figure 3.3.

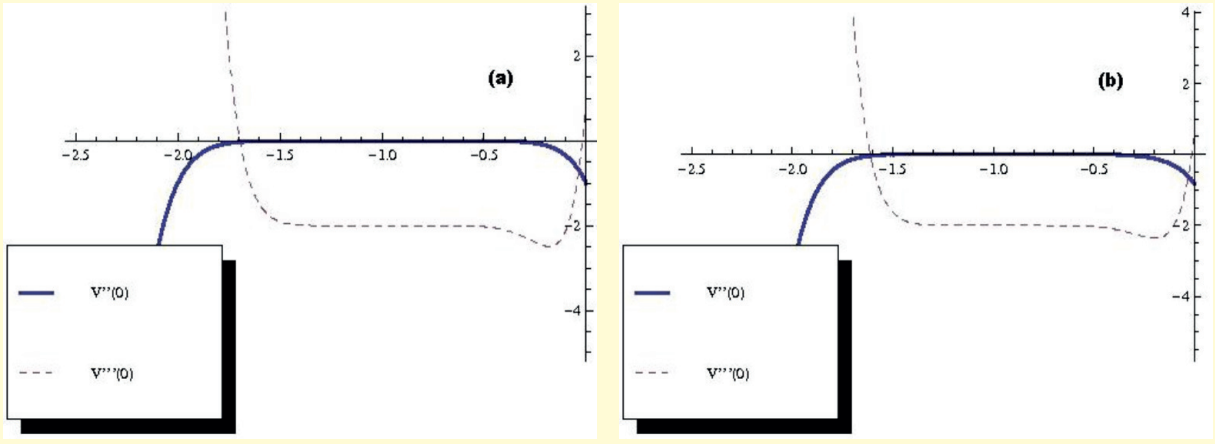

Figure 3.3 Thick line v" (0) Vs h and dotted line v"' (0) vs h, HAM solution up-to 10th order by (a) Liao's scheme, (b) our proposed scheme.

Table 3.4 We have taken convergence control parameter, h = -1 at all orders for both schemes.

t	5^{th} order Liao's scheme	5^{th} order proposed scheme	10^{th} order Liao's scheme	10^{th} order proposed scheme	exact solution
1/4	0.24491	0.24490	0.24492	0.24492	0.24492
1/2	0.46190	0.46184	0.46212	0.46212	0.46212
3/4	0.63420	0.63414	0.63514	0.63515	0.63515
1	0.75964	0.75965	0.76156	0.76159	0.76159
3/2	0.90204	0.90225	0.90507	0.90513	0.90514
2	0.96120	0.96147	0.96395	0.96402	0.96403
5/2	0.98454	0.98477	0.98655	0.98661	0.98661
3	0.99367	0.99384	0.99501	0.99506	0.99505
4	0.99878	0.99885	0.99931	0.99933	0.99933
5	0.99970	0.99973	0.99990	0.99991	0.99991
10	1.00000	1.00000	1.00000	1.00000	1.00000
100	1.00000	1.00000	1.00000	1.00000	1.00000