WP8: Parallel algorithms and GRID applications for computer modeling of processes and phenomena in Micro-Electro-Mechanical Systems (MEMS).

1. Major Activities and Results

Task 8.1: Computer Simulation of micro-gas flows in elements of Micro-Electro-Mechanical Systems (MEMS).

The Direct Simulation Monte Carlo (DSMC) technique was proposed by Graeme Bird in the beginning of sixties of the last century and over the years became a powerful numerical method for studying rarefied gas dynamics and micro gas flow problems. The DSMC technique uses a finite set of model particles denoted by their positions and velocities that move and collide in a computational domain to perform a stochastic simulation of the real molecular gas dynamics. The basic concept of the method is built on a discretization in time and space of the real gas dynamics process and splitting the motion into two successive stages of free molecular motion and binary intermolecular collisions within the grid cells each time step. The heart of the method is the stochastic binary collision scheme. As a result of subsequent theoretical investigations, several collision schemes based on the principle of maximum collision rate per time step have gained popularity: "No Time Counter (NTC)", "Null-Collision", "Majorant Frequency Scheme". The most frequently used scheme has become the Bird’s NTC scheme. Under one or other form this collision scheme presents in the most contemporary applications of the DSMC method that use structured and unstructured meshes with subcells. Two basic problems of the DSMC calculations have been revealed in addition to the inherent discratization problems of the deterministic numerical approaches, namely, the presence of statistical noise in the numerical solution and the dependence of the results on particle number per cell. Until recently no much attention was paid to the second problem. Basically, all collision schemes using principle of a maximum number of particles pairs to be checked for collision require a number of particles (N > 10-20) per cell in order to obtain reliable results. The reason is that all these algorithms by using acceptance-rejection method to calculate the actual number of collisions allow multiple repeat collisions between one and the same particle pair that lead to distortion of the collision process in cells with small number of particles. An alternative way of construction of collision algorithms is proposed by Yanitskiy on the base of the Kac stochastic model of the collision process in a homogenous rarefied gas. It was suggested instead counting the number of collisions within a time step to provide with a probability for collision each particle pair in accordance with the Kac stochastic model and check all pair combinations for collision. The proposed Bernoulli trials scheme has not received wide spread due to the fact that its efficiency depends on the square of the number of particles in cell. However, it avoids repeat collisions and revealed improved accuracy for small number of particles per cell. In this paper we follow Yanitskiy approach and show how to derive efficient collision schemes without repeat collisions from the Kac stochastic model. The results are reported at 28TH INTERNATIONAL SYMPOSIUM ON RAREFIED GAS DYNAMICS 2012, 9–13 July 2012, Zaragoza, and published in [S_12].

The Direct simulation Monte Carlo (DSMC) method in low Knudsen rarefied flows at micro/nanoscales remains a big challenge for researchers due to large computational requirements. In this article, the application of the simplified Bernoulli-trials (SBT)/dual grid collision scheme is extended for solving low Knudsen/low speed and low Knudsen/high gradient rarefied micro/nanoflows. The main advantage of the SBT algorithm is to provide accurate calculations using much smaller number of particles per cell, i.e., <N>=2, which is quite beneficial for near continuum DSMC simulations where the requirement of fine meshes faces the simulation with serious memory restrictions. Comparing the results of the SBT/dual grid scheme with the no time counter (NTC) scheme and majorant frequency scheme (MFS), it is shown that the SBT/dual grid scheme could successfully predict the thermal pattern and hydrodynamics field as well as surface parameters such as velocity slip, temperature jump and wall heat fluxes. Therefore, we present SBT/dual grid algorithm as a suitable alternative of the standard collision schemes in the DSMC method for typical micro/nano-flows solution. Nonlinear flux-corrected transport (FCT) algorithm is also employed as a filter to extract the smooth solution from the noisy DSMC calculation for low speed/low Knudsen number DSMC calculations. The results of this investigation are published in paper [JRNS_13].

The third investigation concerns new potential microfluidic applications of the rapidly emerging industry of micro-electro-mechanical devices. The analysis of the possible flow regimes is an important task of any microfluidic investigation. For a gas flow the transition between steady and unsteady regimes occurs at small Knudsen number Kn < 0.1 (Kn = l_0 / L, where l_0 is the mean free path of the gas molecules and L is the characteristic length). A continuum approach based on the Navier-Stokes-Fourier equations is applicable for this investigation. On the other side, the microfluidic application requires the problem to be investigated starting at very low Mach numbers (M = 0.1), close to incompressible regime. This makes pressure based methods very suitable for this investigation. The system of Navier-Stokes-Fourier equations is calculated numerically using pressure based algorithm SIMPLE-TS.

To study final state of flow past a square in a microchannel as function of Knudsen and Mach numbers have to be calculated series of problems. Each problem requires computational time from 6 to 100 hours run on a 50 to 100 CPU cores. The problems do very intensive calculations and use small amount of memory (8000x100 cells, which is 35MB RAM of a serial code). These fits perfectly to todays vector processors - graphics processing unit (GPU) and motivate us to develop GPU version of the algorithm SIMPLE-TS. Initially in SIMPLE-TS GPU algorithm was implemented first order scheme of approximation of convective terms and density in middle points. The performance of double precision floating point calculations, of flow past a square in a microchannel at supersonic speed M=2.43, on GPU device AMD Radeon HD 7950 is 90 GF/s, which is 1/8th of maximum performance of device (717 GF/s) and is 46 times faster then serial CPU code run on Intel Xeon X5560. The results were reported at the 9th International Conference on "Large-Scale Scientific Computations" June 3-7, 2013, Sozopol, Bulgaria, [1]. The publication [SAS_13a] is accepted.

Additionally in SIMPLE-TS GPU algorithm are implemented second order TVD schemes for approximation of convective terms and density in middle points. The paper [SAS_13p] is in process of preparation.

<u>Task 8.2</u>: Thermo-elastic large amplitude vibration of structures with applications in MEMS and methods for damage detections.

The task includes modeling of the nonlinear dynamic behaviour of healthy and damaged plates, applicable in MEMS as well as methods for damage detection. In the framework of this task a model of the nonlinear dynamic behaviour of layered beam with delamination.

The developed mode is an extension of the existing models of the vibration of beams with delamination. The model takes into account the contact interaction between the sublaminates considering not only the normal forces but the shear forces as well. освен нормалните усилия между слоевете също и появяващите се срязващи такива. Furthermore, the additional damping of the vibrations due to the sublaminate frictions is also taken into account.

A numerical model based on the finite difference approach as regards the space variable and the Gear’s method for solution of ODE as regard the time numerical results was build. Numerical results for the dynamic response of in tact and damaged beam were obtained.

Experimental study was performed in order to verify the results. Laminated beams were produced in the Lab by using glass-epoxy composite and Kevlar. In order to model the delamination small parts of two adjacent composite layers were cut out and replaced by inclusions from different materials, thus modelling the delamination. Teflon, still, titanium and alumina layers were used as inclusions. Using various inclusions aimed to examine the influence of friction between the inclusions on the response of the beam. A modal hammer was used. By this hammer the clamped samples were excited to vibrate and the contact force was recorded. The response of the structures was measured by a laser sensor. Parts of the experimental and numerical results are shown in Figs 1 and 2.

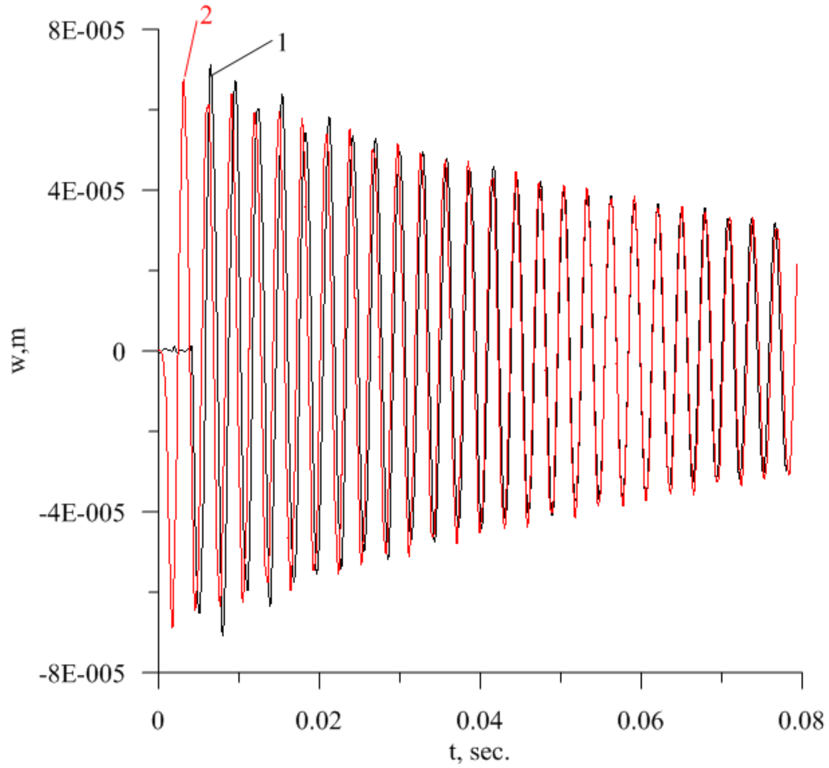

Figure 1. Time history diagram of the beam centre in the case of the Teflon inclusion. 1 (Black colour) – experimental results, 2(red colour) – numerical results. t_0=0.00141 s.

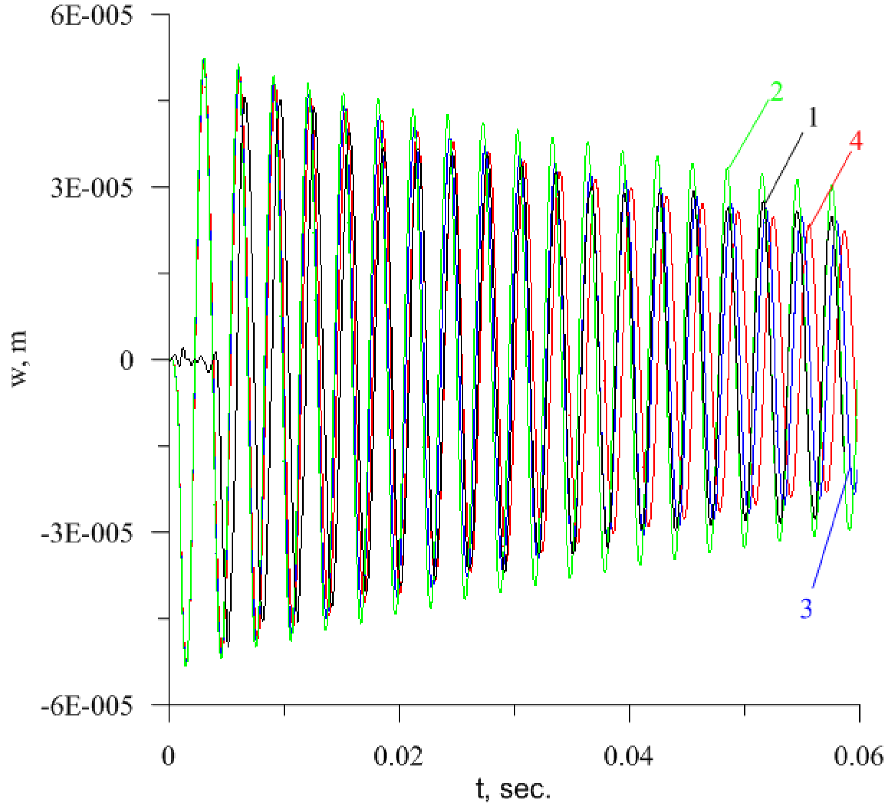

Figure 2. Time history diagram of the beam centre in the case of titanium inclusion. 1 – black color – experimental results; 2 - Green colour – $\bar{c}1_{titanium}$ =0, 3- Blue colour - $\bar{c}1_{titanium} = 0.0015365$, 4- red colour – $\bar{c}1_{titanium} = 0.003073$

From the figures it is clearly seen the very good agreement between the experimental and numerical results. The influence of the additional damping due to the delamination on the response of the beams is also very well expressed (Fig.2). The influence of the location and the length of delamination on the response of the structures are also studied. These results are published in papers in international journals ***Mechanics Research Communications*** и ***European Physical Journal – Special Topics***.
The new model is recently extended by taking into account the geometrical nonlinearity due due to large deflections as well as the temperature influence. The first results were presented at EUROMECH colloquium 541 ”New Advances in the Nonlinear Dynamics and Control of Composites for Smart Engineering Design“ – Senigallia, Italy, 03-06.06.2013. The studies in this direction continue.

Large amplitude vibrations of a Timoshenko beam under an influence of the elevated temperatureis studied in a work presented at 9th International Conference on Multibody Systems, Nonlinear Dynamics, and Control, August 4-7, 2013, Portland, Oregon, USA. It is assumed that the beam gets the elevated temperature instantly and the temperature is uniformly distributed along the beam’s length and cross-section. The mathematical model represented by a set of partial differential equations is derived taking into account boundary conditions for a simply supported beam in the both ends. Next, the problem is reduced by the Galerkin method by means of free vibration modes. The influence of the temperature on a resonance localisation and nonlinear oscillations is studied numerically and analytically by the multiple time scale method. Part of the results are shown in Figs. 3 and 4.

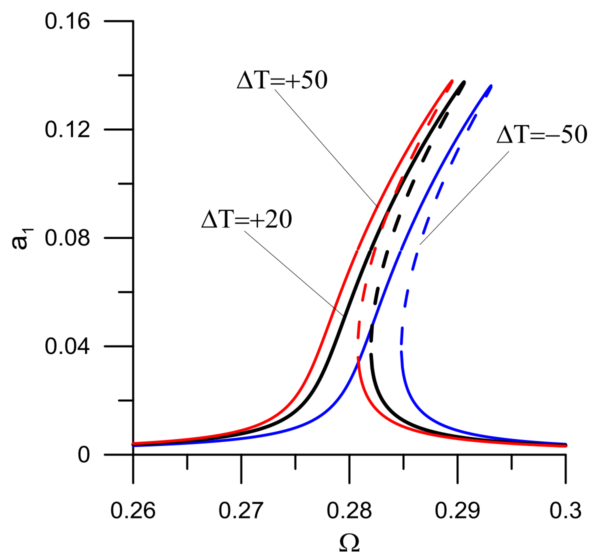

FIGURE 3. Resonance curve calculated for selected values of temperature $\Delta T = -50$, $\Delta T = 20$, $\Delta T = +50$ and fixed mechanical loading $p_1 = 4\times10^{-5}$.

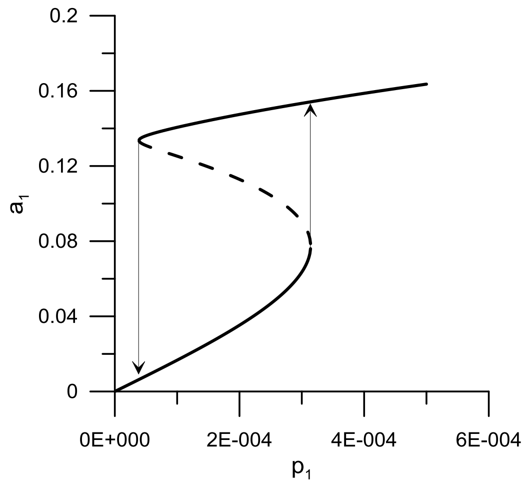

Figure 4. Bifurcation curve versus varied amplitude of mechanical loading and fixed temperature $\Delta T = 20$, excitation frequency (a) ω=0.27, (b) ω=0.29.

At present the developed model is extended by using 3 modes of vibration to reduce the order of the model.

2. Publications with acknowledgements to the project SuperCA++- 2009 No DCVP 02/1

а) published:

[S_12] S. Stefanov, DSMC collision algorithms based on Kac Stochastic Model, AIP Conf. Proc. 1501, 609-615 (2012); doi: 10.1063/1.4769598, ISBN: 978-0-7354-1115-9,

[JRNS_13] A. Amiri-Jaghargh, E. Roohi, H. Niazmand, S. Stefanov, DSMC simulation of low Knudsen micro/nanoflows using small number of particles per cells, Journal of Heat Transfer **135**(10), 101008-1-101008-8 (2013). doi:10.1115/1.4024505

[MWAS-12]E. Manoach, J. Warminski, S. Samborski, A. Mitura, Dynamics of a composite Timoshenko beam with delamination. Mechanics Research Communications. 46 (2012), 47-53,

[MSAW-12] E. Manoach, S. Samborski, A. Mitura, J. Warminski. Vibration based damage detection in composite beams under temperature variations using Poincaré maps. Int. J. Mechanical Sciences, 62 (2012), 120-132.

[WWM-13] Warminska, A., Warminski, J., Manoach , E. Temperature influence on nonlinear responses of Timoshenko beam . *9th International Conference on Multibody Systems, Nonlinear Dynamics, and Control*, August 4-7, 2013, Portland, Oregon, USA. Paper: DETC2013-12624.

[MWAS-13] E. Manoach, J. Warminski, A. Mitura, S. Samborski, Dynamics of a laminated composite beam with delamination and inclusions. *European Physical Journal – Special Topics*, **222**, 1649-1664 (2013)

б) accepted:

[SAS_13a] K. Shterev, E. Atanassov and S. Stefanov, GPU calculations of unsteady viscous compressible and heat conductive gas flow at supersonic speed, 9th International Conference on "Large-Scale Scientific Computations" June 3-7, 2013, Sozopol, Bulgaria.

в) submitted:

г) in preparation:

SAS_13p] K. Shterev, E. Atanassov and S. Stefanov, GPU calculations of unsteady viscous compressible and heat conductive gas flows.

[WWM-13 p] J. Warminski, A. Warminska, E. Manoach. Nonlinear multimodal interactions of a reduced Timoshenko beam subjected to thermal and mechanical loading

3. Presentations and talks

[1] K. Shterev, GPU calculations of unsteady viscous compressible and heat conductive gas flow at supersonic speed, 9th International Conference on "Large-Scale Scientific Computations" June 3-7, 2013, Sozopol, Bulgaria.

[2] S. Stefanov, 28-th International symposium on rarefied gas dynamics 2012, 9–13 July 2012, Zaragoza, Spain.

[3] E. Manoach, A. Warminska, J. Warminski, Large amplitude vibrations of timoshenko beams with delamination in thermal environment. EUROMECH colloquium 541 “New Advances in the Nonlinear Dynamics and Control of Composites for Smart Engineering Design” – Senigallia, Italy, 03-06.06.2013

4. Others

[1] Hardware tests and upgrade of version of operating system of IMECH cluster.