# Coupling Scheme for Continuum and Parallel DSMC Parts to a Numerical Solution of a Two-Dimensional Subsonic Problem

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## Introduction

Many fluid dynamical problems include the regions with very large gradients of macroscopic flow parameters, where continuum assumption may be suspected. Though as a rule these regions are quite small, they have a considerable effect on properties of an application interest and thus it is very important to accurately resolve them. This is also true for problems, which contain as its portion some flow in very narrow channels with linear sizes of molecular mean free path (mfp) order. So continuum assumption is again wrong and one needs for all these flow portions a kind of microscopic description and direct simulation Monte Carlo (DSMC) method introduced by Bird [1] is quite suitable for that purpose. Unfortunally it is rather intensive computationally in comparison with numerical solution of the Navier-Stokes equations. So scientists engaged in computational fluid dynamics (CFD) are making efforts to combine the faster solutions of a continuum approach with the DSMC method in a kind of a hybrid technique. In the part of the flow, where the continuum approach is valid an Euler or Navier-Stokes solver is used and in the remaining usually much smaller parts the DSMC method is employed, with its *cpu* time consumption being accordingly noticeably reduced. But these solutions must be coupled along some space boundaries as well as in their time development. Up to now several different coupling procedures have been introduced. Some of them were discussed by Hash and Hassan in their paper [2] and tested in one-dimensional Couette problem. An adaptive coupling scheme was introduced for hypersonic flows by Le Talles and Malinger [3]. Most of them were intended for aerospace applications, where along with coupling itself it is of importance also that border between coupled solutions should be properly placed.

In this paper it is considered an unsteady problem of the gap flow simulation in the Winchester-type disc drives under transient conditions with some special coupling scheme, which is discussed in the following sections. The coupling of DSMC simulation with this continuum solution is realized as step by step approximation. It is found that the molecular density before and after the channel differs markedly from the atmospheric one because of the slowing down of the flow by magnetic head. Thus previously much used atmospheric pressure boundary conditions are unreal. Space and time distributions of different flow parameters are obtained.

## Statement of the problem

It is considered a two-dimensional simulation problem for flow around the magnetic head and inside the channel, which is formed by the latter with the hard disc moving with constant velocity $U_w$, see Fig.1. In this channel and in the additional regions of $20\lambda$ height and long before and after the head a numerical solution was obtained with the help of DSMC method which was coupled along the boundaries at 0C and CD on the left and GF, FE on the right with a continuous finite element solution of Navier-Stokes equations. The latter produces boundary conditions for DSMC simulations by forming fluxes, which are calculated from mean velocities and its derivatives on these boundaries. Molecular interactions are taken to be the hard sphere one and

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their interaction with the wall was diffuse reflection. The square cells in DSMC computational region had the linear size of approximately $\lambda/3$ and time step $\Delta t$ was less than one third of the molecular mean free time (mft) $\Delta t = 4 \cdot 10^{-11}$. The height of the inlet and outlet in the channel was equal to $2\lambda$ and $\lambda$ accordingly. The initial rotation of the lower wall which models the magnetic media of the disk drive for small time interval can be approximated as being set moving instantly with linear speed $U_w$ from the rest in a direction parallel to itself and thereafter maintained in uniform motion. The speed $U_w$ was taken to be 75m/s, which is representative for the devices of $10^4$ rpm of the media with the 3.5in diameter. The flow itself is formed because of the air molecules after diffuse reflection from this wall are carried along this motion.

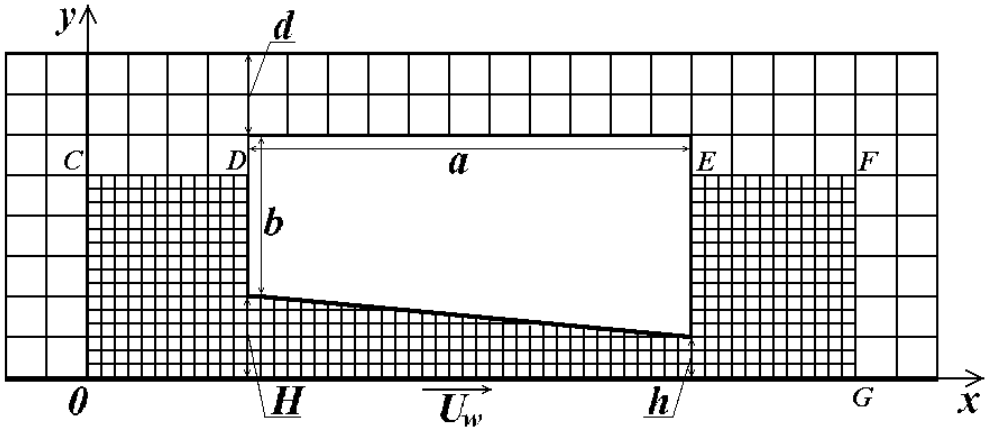


**Fig. 1.** Computational region.

The coupling procedure was realized as a step by step approximation. First in the whole computational region Navier-Stokes equations were solved by finite element method with diminishing cell size in these additional regions and the channel. As the boundary conditions for this solution quite far from the head an asymptotic solution of the Rayleigh problem obtained by Cercignani and et al. [4] was used.

Though employment of continuum equations near inlet, outlet and inside of the channel is inadequate one can expect that on the boundaries 0CDEFG which are $20\lambda$ apart from them the influence of these small bad parts will be insignificant. So, at the next step within this part the DSMC method was employed with incoming molecular fluxes calculated from the stored mean velocities and their derivatives at these boundaries obtained at the previous step. Details of this procedure are outlined in the next section.

## Simulations of the incoming fluxes

The linear size of the cells in finite element solution was four times and its time step was 25 times larger than in DSMC simulation, so that an interpolation of the stored macroscopic parameters was used. Molecular properties in a Navier-Stokes solution are represented through the Chapmen-Enskog velocity distribution function $f(u,v,w)$. Its coefficients $\alpha_i$ and $\beta_i$ contain spatial derivatives of mean velocities and temperature.

$$f(u,v,w) = f_0(u,v,w)\left(1 - (c^2 - 2.5)(\beta_1 u + \beta_2 v) - \alpha_1 u^2 - \alpha_2 v^2 + \alpha_3 w^2 - \alpha uv\right), \quad (1)$$

where $f_0(u,v,w)$ is the Maxwell velocity distribution function, and $c^2 = u^2 + v^2 + w^2$

$$f_0(u,v,w) = \pi^{-3/2} \exp\left[-\left(u^2 + v^2 + w^2\right)\right].$$

As in our problem there is no boundary temperature differences in the data and all mean velocities are relatively small in comparison with the sound velocity $a_s$ ($a_s$=320m/s) we have neglected the temperature derivatives, the coefficients $\beta_i$, in $f(u,v,w)$. Simulations confirmed this assumption and the corresponding evidence will be presented later on in the paper. So with

decart thermal velocity components $u=(u'-u_{av})/V_T$, $v=(v'-v_{av})/V_T$, $w=w'/V_T$ being related to the most probable velocity $V_T$ , $V_T^2 = 2kT/m$, where $m$ is the molecular mass and $k$ – Boltzmann's constant, it can be represented in a simpler form:

$$f(u,v,w) = f_0(u,v,w)\left(1 - \alpha_1 u^2 - \alpha_2 v^2 + \alpha_3 w^2 - \alpha uv\right), \quad (2)$$

And coefficients $\alpha_i$ are obtained from mean velocities and their derivatives on the boundary 0CD and EFG (cl. Fig.1 ) of finite element solution at different time moments and stored in special file. Afterwards they are red during DSMC simulations and used for simulating boundary incoming fluxes inside the DSMC computational.

## Numerical Evaluation of the Present Coupling Scheme

Convergence of the step by step approximation used in the present paper for coupling of two solutions was evaluated by comparison of successive approximations for mean velocity components $u_{av}$ and $v_{av}$ as well as for density $n_{av}$ at the boundary 0CDEFG (cl. Fig.1). The relative differences of zero approximation $u^0_{av}$ as obtained from the finite element solution and the first one $u^1_{av}$ after DSMC simulations $Ru=(u^0_{av}-u^1_{av})/u^1_{av}$ and in the same way for $Rv$ and $Rn$ are shown on the Fig.2 and Fig.3. inevitably at particular time moment. But as a matter of fact for the other times the whole picture is roughly the same. The relative differences for X-velocity component $Ru$ as shown on the left in Fig.2 oscillate near a zero level with peak-to-peak values mostly less than 10% but somewhat grow between $26<N_c<50$ where the component $u_{av}$ is itself small so that statistical scattering becomes larger being apparently the origin of it.

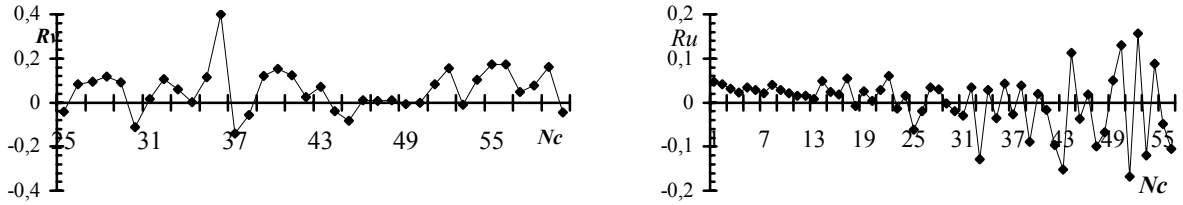


**Fig. 2**. Relative differences $Ru$ and $Rv$, composed from successive approximations.

The relative differences for Y-velocity component $Rv_{av} = (v^0_{av} - v^1_{av})/v^1_{av}$ are shown in Fig.2 on the right. Their chaotic oscillations near zero level with peak values amount to 30%. As the $v_{av}$ magnitude is mostly much less than that of $u_{av}$ , it can be explained again by statistical scattering. The relative density differences $Rn_{av}=(n^0_{av}-n^1_{av})/n^1_{av}$ are shown on Fig.3. It is clearly seen that they vary near the 1%-2% level of precision with peak-to-peak values of about 3%.

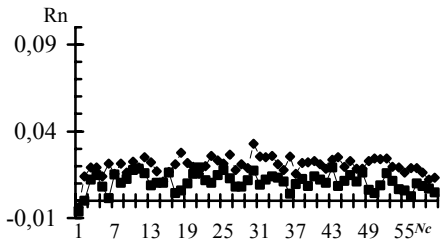


**Fig. 3.** Relative density differences.

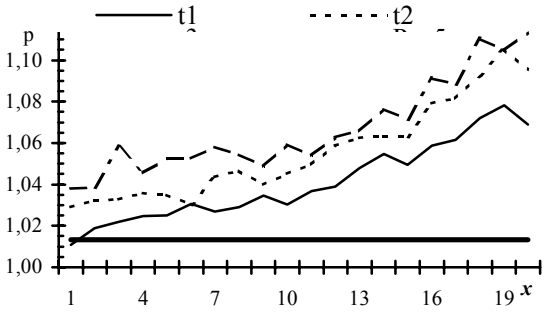


**Fig. 4**. Pressure $p$ before the channel inlet.

Thus one can say that except the random statistical scattering inherent to DSMC method the mean level of these relative differences does not exceed 10%. So that convergence of this step-by-step coupling approximation is satisfactory.

## Some numerical simulation results

Simulations for our DSMC parallel code were performed on the St. Petersburg university clusters. The largest of them contains 40 processors Intel Pentium III 933 MHz. Parallelization of the code was proceeded through independent realizations when each processor produced the whole solution, the results being gathered then on some leading one for averaging and outputting. This scheme allowed us sometimes use an additional cluster located far away but connected with one of the ours through the Internet channel into a metacomputer with good efficiency, for details see [5]. All previous researchers [6-8], have used the assumption that before the inlet and after outlet of the channel unperturbed atmospheric pressure could be used as the boundary condition. Thus they entirely neglected the slowing down of the flow by magnetic head. We are now in a position to check it.

For this purpose during simulations particle density before and after the channel has been determined and pressure $p$ was calculated by ideal gas relation $p=nkT$. On the Fig.4 it is represented for the height $y=\lambda/3$. There a horizontal bold solid line represents atmospheric pressure, the solid curve is the pressure for time $t_1=10^{-8}$s, dotted one for time $t_2=10^{-7}$s. and dashed for $t_3=5*10^{-7}$ s. It is clearly seen that the slowing down of the flow is present by a 8% increase in pressure before the channel inlet. After the outlet the pressure is on the contrary much lower than the atmospheric one. Thus one may conclude that the pressure boundary conditions used in previous papers at least for $U_w \geq 75$m/s are not fulfilled. Both of the pressures before and after the magnetic head are not atmospheric and are quite different near the inlet and outlet.

## Conclusions

The present coupling scheme of the DSMC method with a continuum solution at the outer regions proves to be convergent. With its help we have found considerable deviations from the atmospheric pressure before and after the channel. Thus quality of the pressure boundary conditions much used in the previous papers on this topic seems to be doubtful. Space and time distributions of different parameters of the flow are also obtained.

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