An Investigation of Asperity Contact in a Slider Air Bearing by a Three-Dimensional Direct Simulation Monte Carlo Method

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Abstract

A direct simulation Monte Carlo (DSMC) method is used to solve a slider air bearing problem when isolated contacts occur. A flat slider with a spherical asperity underneath is simulated when the tip of the asperity has a point contact with a plate moving at constant speed. Two-dimensional air bearing pressure profiles are obtained by using the ideal gas law. The air bearing force on the slider is obtained by calculating the time-averaged change in the vertical momentum of the simulated particles striking the slider. The results show that the pressure is bounded at the contact point. A vacuum region around the contact point is added in the simulation that is too small for a molecule to enter. The results also show that the peak pressure and the resultant force converge as the calculation grid gets denser.

I. INTRODUCTION

Read/write head sliders in computer hard drives are flying lower and lower above the disk surface in order to increase the magnetic recording density. The slider air bearing modeling used to obtained the air bearing force and flying height prediction is crucial in slider air bearing design, and it is necessary to increase the accuracy of calculation for flying heights less than the local mean free path of the gas molecules (65 nm at STP for air).

Traditionally, macroscopic hydrodynamic equations (e.g. Navier-Stokes, Reynolds) have been used to model slider air bearing problems. However, when the Knudsen number Kn > 1, where Kn is defined as the ratio of the molecular mean free path to the characteristic length of the flow, the flow may not satisfy the non-slip condition on the solid boundaries [1]. The Molecular Gas-film Lubrication (MGL) model [2], which is currently widely used in the hard drive applications, is the Reynolds equation with the slip correction based on the Boltzmann equation where the Poiseuille flow rate is calculated on the basis of a linearized BGK model of the Boltzmann equation. Even though the MGL model still treats the gas inside the region as continuous, except on the boundaries, in a previous study, this model was shown to work well for large Knudsen numbers [3], [4].

In most cases, isolated contact can not be avoided in the slider air bearing as the slider flies lower and lower. The introduction of the laser bump in the landing zone, which is designed to avoid stiction, also requires the knowledge of bump contact physics. However, the MGL model predicts unbounded pressure at the contact points [5], [6] and therefore, strictly speaking, cannot be used to obtain steady state or dynamic solutions of the contact air bearing

problems. In [6], the order of the contact singularity is studied by simulation of a contact asperity with a shape of a *cosine* function. It is shown that ph approaches a constant at the point of contact, where p and h are pressure and spacing, respectively. They also showed that in most cases, $h \propto o(r^{-2})$, where r is the distance from the contact point, and the singularities in p are not integrable. Therefore, the forces predicted by the Reynolds equation with various slip correction models are also unbounded, and these models evidently can not be used to understand the real contact physical situation for slider air bearings.

The direct simulation Monte Carlo (DSMC) method was developed in the late 1960's by G. A. Bird [7]. It has been tested thoroughly since and found to have excellent agreement with both molecular dynamics solutions and experiments. DSMC has been applied to the slider air bearing problem successfully by Alexander, *et al*. [3], Huang, *et al* [4] and Fukui, *et al* [8]. In [3], the results for a two-dimensional flat slider are compared to the MGL results, they are shown to be in good agreement. The verification of the MGL model was extended to three-dimensional problems in [4] and in addition, the first calculation of an air bearing with line contact was presented. It was shown that near the contact line, the pressure drops to zero.

The DSMC method simulates the gas molecules inside the head/disk interface (HDI). Hundreds of thousands of simulated particles move and collide with each other and the solid boundaries. Their three velocity components and three spatial coordinates are calculated. There is no two-dimensional flow assumption as in the MGL model and the simulation does not depend on the Knudsen number. Particularly when contacts occur, DSMC has the advantage of providing a finite pressure profile and a finite loading force as shown in [4].

Even though DSMC is much faster than the molecular dynamics approach, it still requires large amount of CPU time and memory. For example, it took a week or so to complete

a calculation with 250,000 particles and 10,000 cells on a IBM RS/6000 590 workstation. In most cases, the calculation is much bigger and each current calculation could take months to complete. Therefore, we abandoned the idea of sequential programming and used a parallel supercomputer to increase the speed. Results that were “impractical” to obtained by a serial program before can be obtained in a week by a parallel program.

This report is a continuation of [4]. We simulated a three-dimensional flat slider with a spherical asperity bump underneath. The slider flies over an infinite plate moving at a constant speed. The steady-state pressure profile and the loading force are obtained in the case where the asperity bump touches the moving plate surface.

II. DSMC METHOD AND PARALLEL PROGRAM

A. DSMC Method

Unlike the molecular dynamics model, DSMC does not calculate the instantaneous state of a simulated particle. It only provides probabilities and average quantities. Each particle used by DSMC represents a number of real molecules that are roughly at the same position with roughly the same velocity. The gas under the slider is assumed to be dilute so that the interactions between particles are modeled as two-body collisions and the potential energy of the particles is negligible compared to the kinetic energy. The collision between two particles is assumed to be fully elastic according to Bird's hard sphere molecule [7].

The simulation region is divided into cells that are a fraction of the size a cubic mean free path. These cells are used to process collisions between particles. Only those particles in the same cell can be selected as collision partners, regardless of their positions within the cell. The time step is chosen to be one fifth of the minimum time a particle needs to travel through a single cell with the most probable velocity (337 m/s for the argon atom at STP).

In the simulation, $\{\mathbf{r}_i, \mathbf{v}_i\}$ (i = 1, 2, 3), which are the position and velocity components, are calculated and recorded at each time step. To get the averaged quantities, such as density, temperature, momentum or kinetic energy, the program does the sampling after the flow system reaches its steady state. The steady total number of particles inside the system is proven to be a good indicator of the steady state.

The pressure profile is obtained by applying the ideal gas law to each cell. The air bearing force is calculated as the time-averaged change in the vertical momentum of particles that collide with the slider during the sampling time.

B. Parallel Programming

Because of the size of DSMC calculation, parallel programming is necessary. Parallel computing basically consists of the following: (i) breaking up the task into smaller tasks, (ii) assigning the smaller tasks to multiple processors for simultaneous work and (iii) coordinating the processors. In our study, part (iii) is accomplished by using the so called Message Passing Interface (MPI)

MPI was specified by a committee of about 40 high performance computing experts in a series of meetings in 1993-1994 [9]. It is intended to be a standard message-passing specification that each Massively Parallel Processor (MPP) vendor implements on their system.

Each processor used in the parallel computation is numbered from zero to *numprocs*-1, where *numprocs* is the total number of the processors used and is specified by the user. Processor zero is normally called the *master processor*. The rest of the processors are called the *workers*. Both the master and the workers receive the same copy of the code. The code is written to instruct each processor when and how to do its own calculation and communicate with each other.

The master processor reads data from the hard disk, generates particles and broadcast this information to the corresponding workers. The simulation region is evenly divided into a number of sub-domains and each sub-domain along the length direction is assigned to a single worker by the master. When a particle travels to a sub-domain belonging to another worker, a

message, including the leaving particle's spatial position and velocity, is sent to the corresponding worker. In our program, the master also does simulation just as other workers do. So in this sense, the master is also a worker. The processor *zero*, which is the master, enforces the boundary conditions at the inlet while the processor *numprocs*-1 enforces the boundary conditions at the outlet. Each processor enforces the side boundary conditions of its own region. When the simulation is done, all workers send their results to the master processor for the data analysis and the master is responsible for writing results to the hard disk.

III. DSMC SIMULATION AND RESULTS

Figure 1 shows the 3-D flat slider with a spherical asperity underneath. The height of the figure is exaggerated. The length L of the slider is 4 μm, its width W is 3.3 μm. The base radius of the spherical bump on the slider is 300 nm and the height is 20 nm. The tip of the bump contacts the disk surface at a single point. The distance between the contact point and the slider trailing edge is 1 μm. In this case, the flying heights of the leading edge and trailing edge are about 50 nm and 10 nm, respectively. The plate travels at U = 25 m/s. The pitch angle α is 0.01 rad. There is no skew.

The gas is chosen to be argon with temperature T_0 = 0 °C, density ρ = 1.78 kg/m^3. Argon is chosen in place of air in our study because a single element gas is simpler in the DSMC method. Since the Mach number is low and the Knudsen number is high, the flow field is nearly isothermal. While argon has a different heat capacity from a nitrogen-oxygen mixture due to the fact that it does not have rotation, this difference is not important in isothermal flows. In addition, the molecular mass and diameter of argon are similar to those of nitrogen and oxygen. Therefore, argon is a good candidate for simulating air without considering the molecule's rotation.

Due to the symmetry of the flow and the system geometry, only half of the system is calculated. The plane of symmetry is treated as a fully elastic wall.

The pressure boundary conditions are enforced at the inlet, outlet and along the side by a self-adjusting algorithm [3]. This algorithm adaptively adjusts the velocities of the particles fluxing from the ambient exterior into the system so as to maintain ambient pressure at these boundaries.

The cells are rectangular. The *effective cell volume* is defined as the volume of the part of the cell inside the flow. This volume is needed by the collision algorithm and for calculation of the number density. In this study, the volumes of those cells that intercept with the spherical bump are calculated numerically by integration. The grid used for integration is adaptive such that a smaller cell has a finer grid.

All the DSMC simulations were run on the IBM SP-2 supercomputer at the Maui High Performance Computing Center in Hawaii. The CPU time is about 7 days for a specific case using 16 processors with grid size 3x360x200 and 1.2 million particles.

In the beginning of the DSMC simulation, some "singularity" problems were encountered. Many simulated particles accumulated in a very small region near the contact point. This phenomenon became more severe when more particles or more cells were used. Another "singularity" occurred in the neighborhood of the contact region, where some particles just bounced up and down between the slider and the disk thousands of times in one time step. It took an unlimited amount of CPU time to process these motions. To solve these problems, we created a "non-fly-zone" around the contact point (see Fig. 2) based on the assumption that gas molecules have finite volumes. The boundary of the non-fly-zone is modeled as a vertical circular cylinder centered at the contact point. The radius of this cylinder is such that the height of the cylinder between the spherical bump and the disk surface is about the diameter of an argon atom. When a particle hit this cylinder, it will act like hitting a fully-elastic wall. This prevents any molecules from entering this zone. The pressure in this zone is automatically zero.

Figure 3 shows a pressure profile in the head/disk interface. Clearly seen is a pressure spike in the vicinity of the asperity. Pressure builds up in front of the spherical bump and

reaches a peak with a finite value. Behind the bump, there exists a region with sub-ambient pressure. The detailed structure of the pressure near the contact point can be seen in Fig. 4. The curves on this figure are pressure profiles along the centerline of the slider. The same slider without the spherical bump flying at the same height was simulated and its pressure along the centerline was also plotted as a dotted line for reference. The two curves are very similar far from the contact region. In the contact case, the pressure builds up faster than in the non-contact case near the contact region. This pressure reaches a peak value that is several times atmospheric pressure. The discontinuity of the contact pressure is due to the existence of the "non-fly-zone". Beyond the asperity the pressure increases continuously and merges with the non-contact pressure near the outlet.

Table I lists simulations with different meshes. The case with no asperity is also listed as a reference. The first column of Table I is the number of cells used in the vertical, length and width directions, respectively. The second column is the simulated particle numbers used initially. The peak pressure is the maximum pressure located in front of the contact point. The loading force is the difference between the air bearing force on the lower side of the slider and the atmospheric force on the upper side of the slider. The air bearing force is calculated by averaging the total change of vertical momentum of the particles striking the slider. From Table I, it can be seen that the peak pressure increases as the mesh becomes finer. The value of the peak pressure with cell number 3x360x200 is about 80% larger than in case 3x80x60. The loading force also increases as the mesh becomes finer. But the value for case 3x360x200 is only 4.7% larger than in case 3x80x60. This shows that cell size has less effect on the loading force calculation.

The peak pressure and the loading force as a function of the number of cells used are plotted in Fig. 5 so the trend can be easily seen. All values are normalized by values for the case 3x80x60. Even though the peak pressure has not quite converged in the largest system, it shows a definite trend toward convergence as the mesh is made finer. More cells and particles are needed to get the converged peak pressure. On the other hand, the loading force is consistent in all four cases. This force is in the neighborhood of 0.44 μN and is about 12% larger than that corresponding to the case without the asperity.

The non-dimensional radius of our spherical asperity is about 0.075. From Fig. 3 we can see that the non-dimensional radius of the area affected by the asperity is about twice that size.

IV. CONCLUSION

A good understanding of the physics of asperity contact in the slider air bearing is needed to provide a database for contact modeling and to help improve the air bearing design programs. In our study, the contact problem of a spherical asperity underneath a 3-D flat slider was simulated by using the direct simulation Monte Carlo method. A physically meaningful additional condition was added near the contact point to prevent "singularities". Around the contact point, in a small zone where the length scale in this zone is less than the diameter of the molecules, the pressure was set to zero to model the real situation, since no molecule would be small enough to enter this zone and provide pressure. With this condition no singularities were encountered. The pressure has a jump at the contact point from about twelve times ambient pressure to sub-ambient pressure. In our case, the contact asperity provides 12% larger loading force than the case without the asperity.

DSMC is shown to be a good approach for contact asperity problems. All the results are bounded and tend to converge as the cells get smaller even when there are isolated contact. This is in contrast to the Reynolds equation, which predicts unbounded pressure and force as the spacing approaches zero.

The efficiency for using DSMC is improved dramatically when used with parallel programming since the problem itself we simulate on the computer is a parallel process. In another words, each sub-domain can be calculated independently during one time step. Only slightly less than 1% of the particles move from processor to processor and this means just a small amount of time required to do the message passing.

In most cases, the shape of the asperity can be modeled as a spherical surface. Therefore, the pressure obtained in this report can be implemented in the current air bearing simulation program to calculate the air bearing force when asperity contact occurs.

Reference

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TABEL I

PEAK PRESSURE AND LOADING FORCE

Number of cells	Min. Number of Particles	Peak Pressure P/P_0	Loading Force (μN)
3x80x60	250,000	6.34	0.422
3x120x80	300,000	9.79	0.437
3x240x140	500,000	11.14	0.440
3x360x200	1,200,000	11.58	0.442
No Asperity	250,000	2.0	0.395

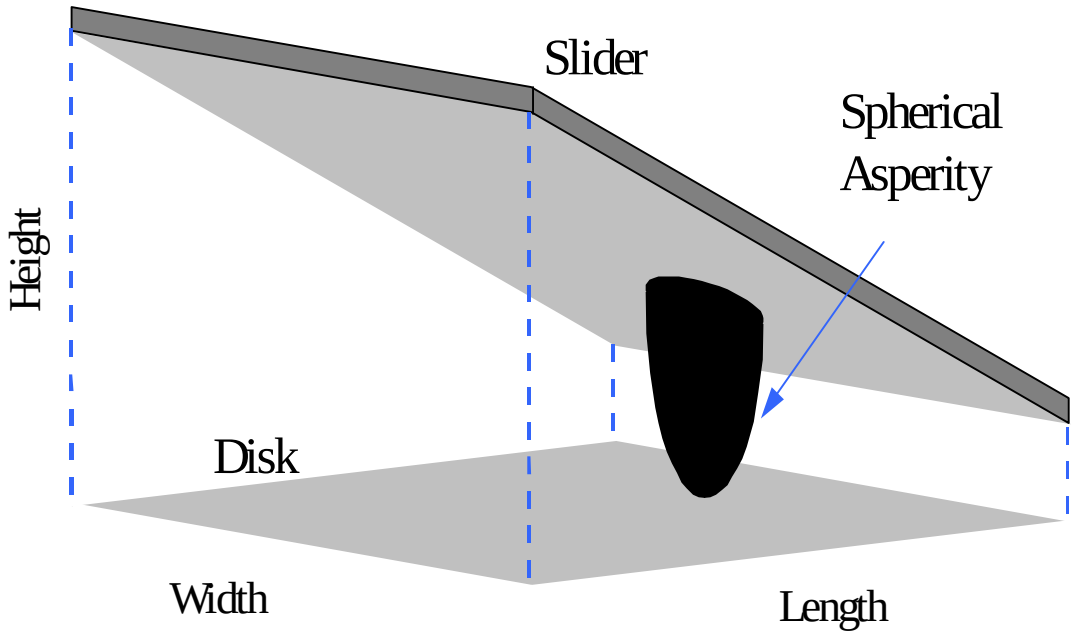

Fig. 1 Flat Slider with a Spherical Asperity

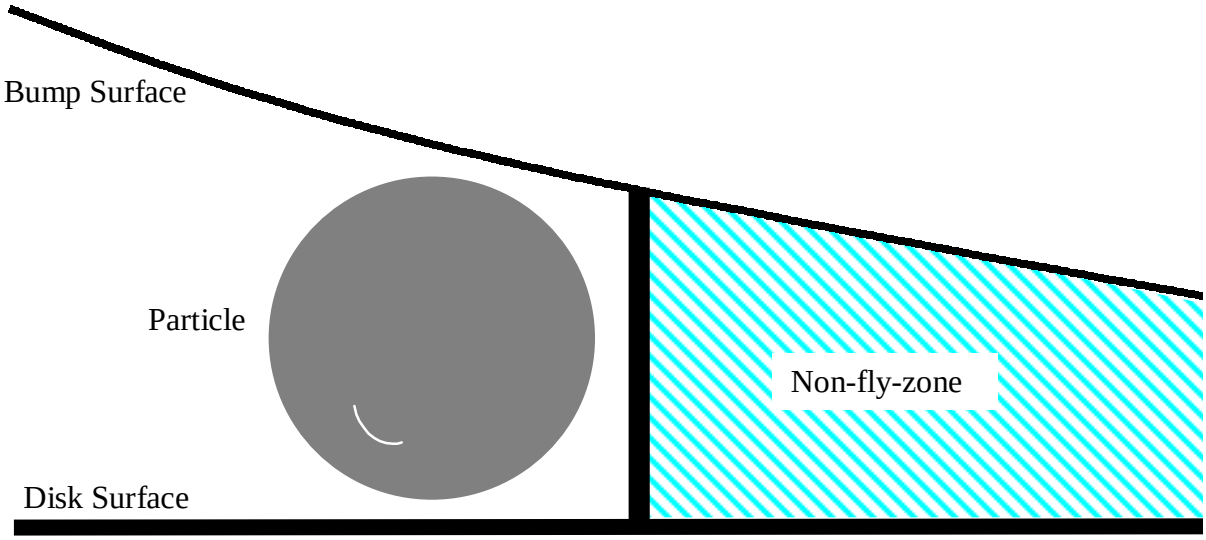

Fig. 2. The non-fly-zone near the contact point

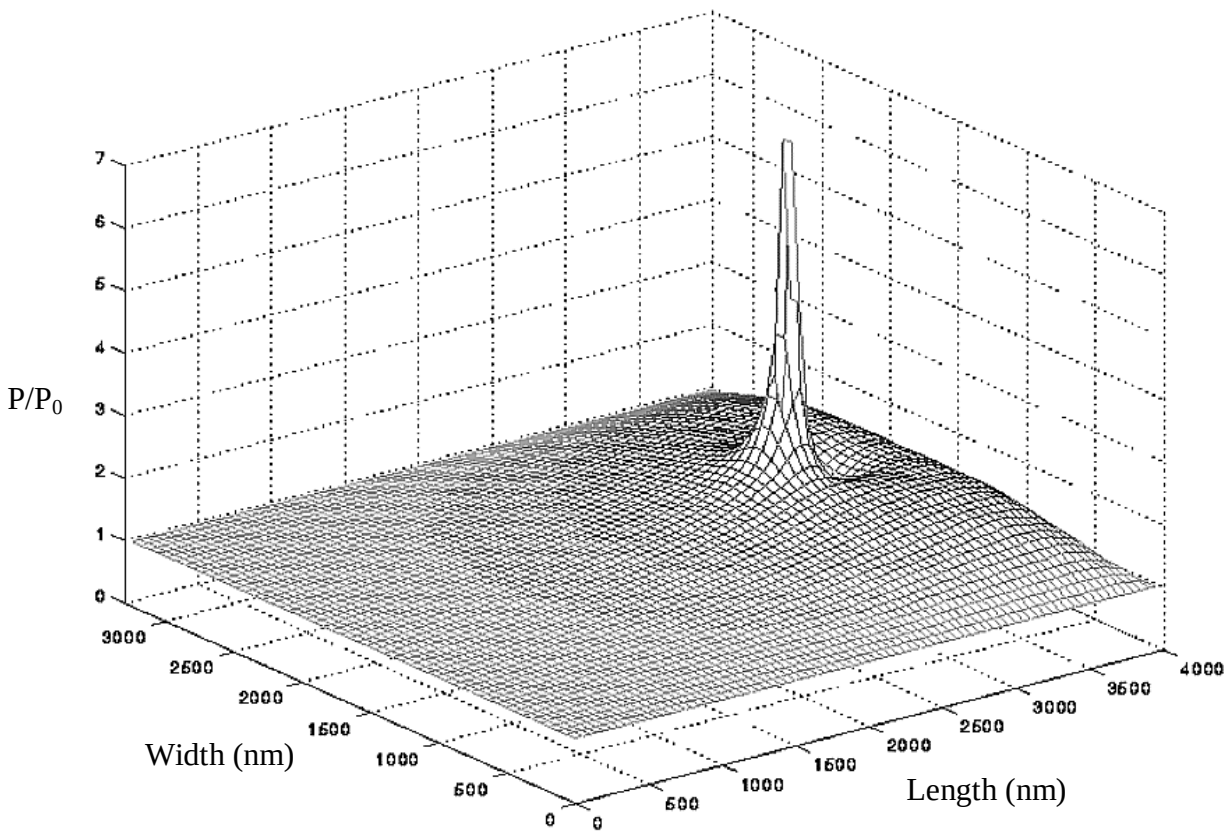

Fig. 3 Contact Pressure profile for the slider with a spherical asperity

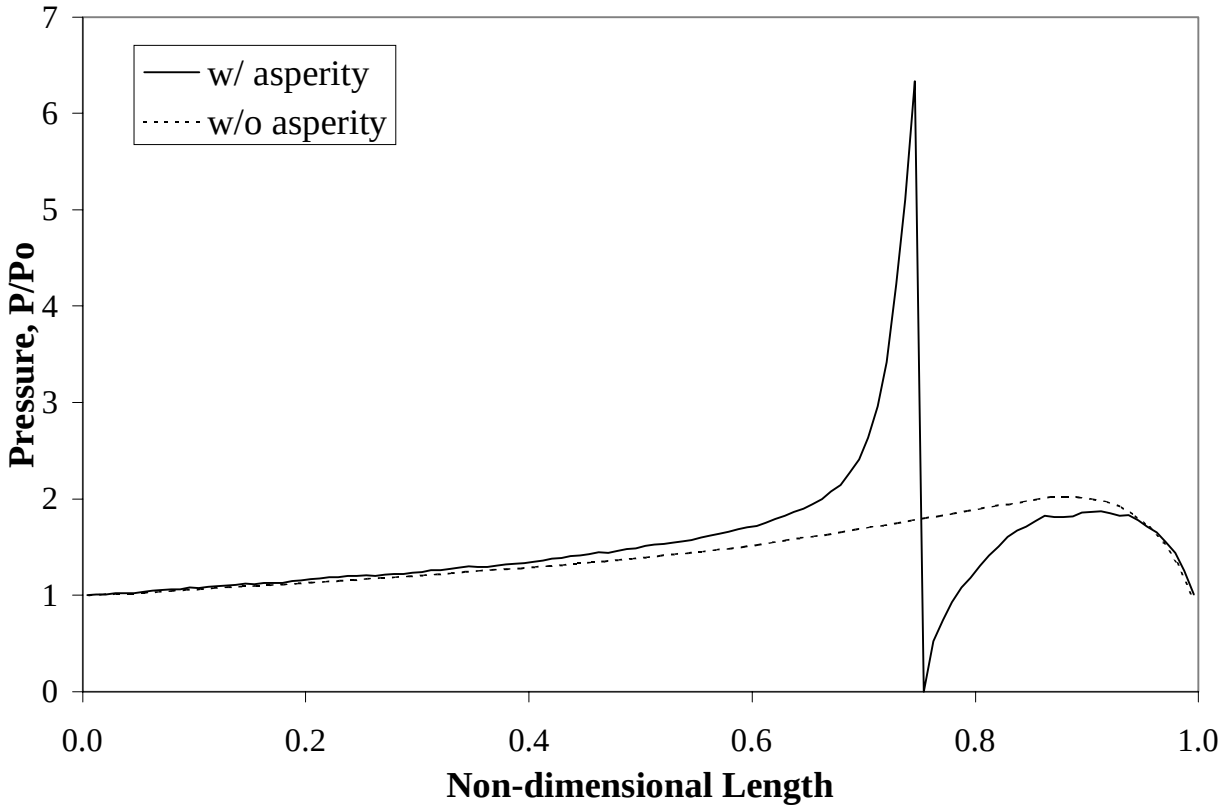

Fig. 4 Pressure along the Centerline of the slider

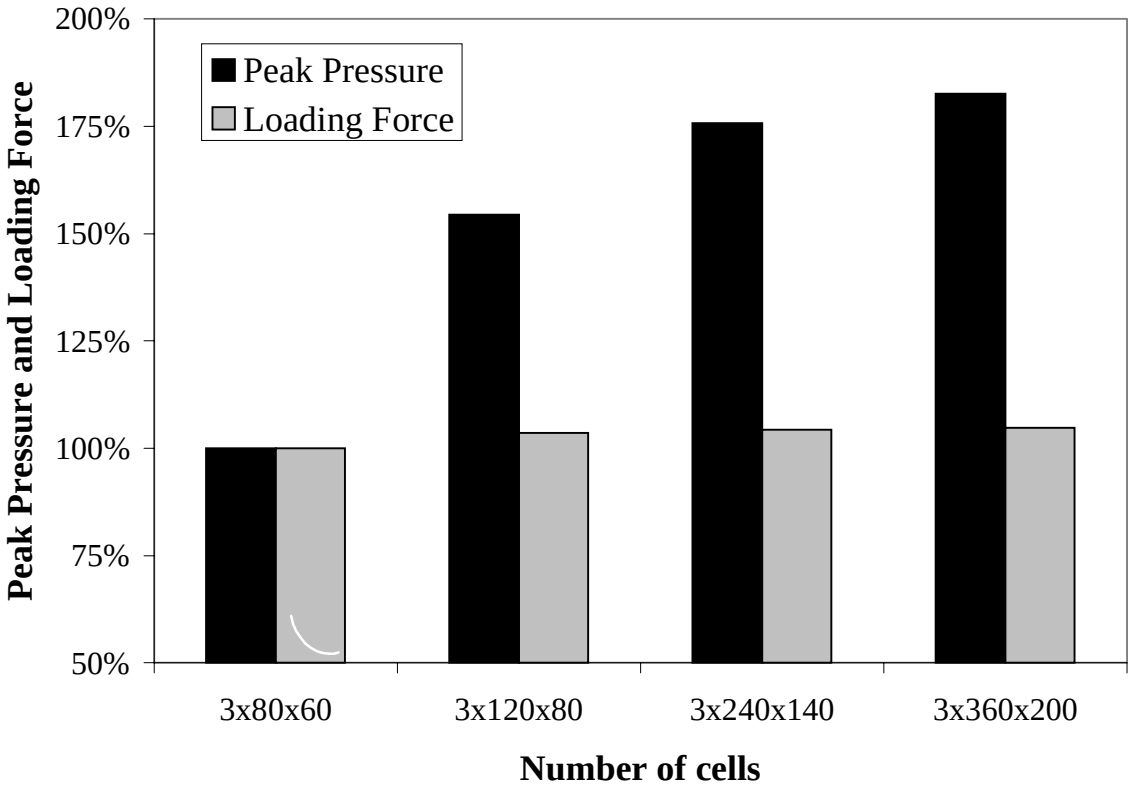

Fig. 5 Peak Pressure and Loading Force as a function of mesh size