DISTRIBUTED SIMULATION of TRANSITIONAL NANOSCALE CHANNEL FLOWS by a DSMC METHOD with an ENHANCED RELIABILITY.

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Summary By distributed simulations on several parallel clusters low flow velocities were resolved. Through application of a hybrid technique important features of a complex channel flow for Winchester-type disc storage devices were established. The two new developed fault tolerant algorithmic procedures for diminishing bad consequences of possible node and link failures increased reliability of such distributed simulations and were applied to a filter problem simulated by a metacomputing scheme.

INTRODUCTION

Many fluid dynamical problems include the regions with very large gradients of macroscopic flow parameters, where continuum assumption may be suspected. This is also true for problems, which contain as its portion flow in very narrow channels, with some of its linear size being of molecular mean free path order. So for all these flow parts a kind of microscopic description is needed and direct simulation Monte Carlo (DSMC) method introduced by Bird [1] is quite suitable for this purpose. Unfortunally it is rather intensive computationally in comparison with numerical solution of the Navier-Stokes equations. The 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. But these solutions must be coupled along some space boundaries as well as in their time development. Such coupling for a simulation, which incorporates quite different scales, was elaborated in the paper for the practically very important problem of flow simulation in future magnetic disc storage devices of Winchester-type. The other difficulty for channel flows in some cases is small values of mean gas velocities in comparison with thermal molecular speeds, which demands large statistical samples and could be overcomed only by using large parallel clusters or joining several of them into a distributed computational system by metacomputing or Grid. In the paper such a problem was considered for two-dimensional flow and rather low flow velocity were resolved with the help of a metacomputing scheme. At the same time a specific problem, related to trouble-free operation of a some body else remote hardware technique, which always comes into play in such occasion, was solved with the help of two new developed fault tolerant algorithmic procedures implemented in the program. They are shown to produce an enhancement of the reliability for Monte Carlo simulations, only partly diminishing the total statistical sample in the case of a computer breakdown in any cluster. They could be easily built in some other user programs. If in user application additionally a check pointing is provided the sample losses are diminished considerably.

GAS FILM LUBRICATION FOR WINCHESTER-TYPE DISC DRIVES

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. The coupling of DSMC simulation with a continuum solution is 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 some additional regions nearby and inside of the channel. As the boundary conditions for this solution, quite far from the head, an asymptotic solution of the Raleigh problem obtained by Cercignani and et al. [2] 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 20λ apart from them the influence of these small bad parts will be insignificant. So, at the next step, within this part the DSMC method [3] was employed, with incoming molecular fluxes calculated from the stored mean velocities and their derivatives at these boundaries obtained at the previous step. The latter procedure utilizes Chapmen-Enskog velocity distribution function. Details of this procedure, which is a kind of transformation of macroscopic information into a statistical microscopic one, are thoroughly elaborated in the paper. Comparison of the relative differences in flow parameters at the boundaries has confirmed good convergence of the method. 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 neglecting this effect appeared to be unreal. Space and time distributions of different flow parameters are obtained. A new developed surface roughness model is now under implementation in the program and its results for accounting surface roughness effects on the flow will be presented to the congress.

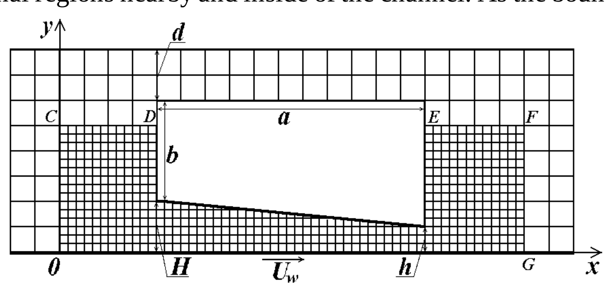

FIGURE 1. Computational region.

DISTRIBUTED SIMULATION OF A TWO-DIMENSIONAL CHANNEL FLOW WITH AN ENHANCED RELIABILITY.

It is considered the flow through two-dimensional infinite in Z-direction channel, which connects two reservoirs with the same gas, the particle densities of them being n1 on the left and n2=0.8n1 in the right. Molecular interaction assumed to be the hard sphere one and their interaction with the channel walls is taken to be diffuse reflection. At the both of the reservoirs temperatures and Maxwell velocity distribution functions were considered to be the same and not perturbed by outgoing streams. The channel width was changing from $\lambda/5$ to 5λ, where λ is mean free path under atmospheric density n1. With the help of DSMC method we were computing profiles of the mean velocity and density inside the channel and some other parameters. Large statistical scattering, producing the error r_N , is a standard difficulty in all applications of the Monte Carlo simulations but it is especially severe for flows with small values of mean gas velocities relative to the thermal molecular speeds. The statistical error r_N in this filter problem, which is just of this

$$r_N = x[D(u)/N]^{1/2} \tag{1}$$

kind, with the variance being $D(u)=0.5V_T^2$, V_T - thermal most probable velocity, and x is equal to 0.6745 for the so called probable error, has been strongly diminished by enlarging the computer number and the samples ***N*** through Internet-connection several clusters into a metacomputer. Separate parallel MPI implementations of the DSMC method for this problem were employed on three clusters, which were operated under different nets: 100Mb/s Ethernet, 1Gb/s SCI and 1Gb/s Myrinet. All of them had distributed memory, two of them being linked into a local net by 100Mb/s channel, the Internet connection with the third cluster "Paritet" of Institute for High Performance Computing was realized through 1Mb/s Internet channel, which nevertheless sometimes showed much lower real performance, especially for transference of relatively large files. Each processor of the whole system produced independent realizations; the results were sent to the corresponding leading one and then gathered at one of latter's for averaging and outputting. Earlier it was developed an efficient dynamic load balance technique [4] for such distributed simulations. Yet computer breakdowns, which were not so seldom, compelled to do something new. And the new developed algorithmic procedure to enhance the reliability of such metacomputing scheme includes the following steps. First, for monitoring the states of the processors participating in a simulation it is necessary to know the information on the nodes obtained in all of clusters. So every script starting a simulation on a cluster simultaneously transmit its node information to the others. Second, every processor after fulfillment its task opens special control file with an extension ***.myrank*** in order to allow for one of them to check with the command ***.*wc –l..*** whether he is the latest. If it is so it checks with another system command ***fping*** the states of all other cluster processors. This operation is performed at all clusters. Then all computational results are gathered (MPI_REDUCE) on the two mains for joint processing and outputting, if no error were detected. Else simulation automatically goes over to an emergency branch where all communications between the misfortune cluster and the others are terminated and its contribution to final statistical sample is lost. A quantitative evaluation of the efficiency of this procedure was obtained, showing that it will be quite valuable for Grid computing with many clusters used for calculations. This is most simple version of the developed procedures. More elaborated version with lesser losses needs much more space for description and will be postponed for the full paper.

CONCLUSIONS

By distributed simulations on several parallel clusters rather low flow velocities were resolved. Through application of a hybrid technique for coupling different computational scales important features of a complex channel flow, which models the flow in Winchester-type disc storage devices, were established. The two new developed fault tolerant algorithmic procedures for diminishing bad consequences of possible node and link failures in this complicated computational systems essentially increased reliability of such distributed simulations and were applied to a filter problem which was simulated with the help of a metacomputing scheme.

References

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