Simulating Microfluidic Devices on Parallel Computers

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The rapid progress in fabricating and utilising Micro-Electro-Mechanical-System (MEMS) during the last decade has led to the fast growing interests and researches in micro-scale fluid dynamics. Alongside of experimental studies, theoretical and computational studies are essential in the understanding of the flow characteristics in micro-scale. A computational fluid dynamics (CFD) package, THOR, was developed in Daresbury Laboratory to study the rapid mixing and reaction in micro-channels and capillaries and slip flow past a sphere.

THOR can deal with complex geometry with multi-block grids of body-fitted coordinates. The basic idea is to use a curvilinear coordinate transformation to map the complex flow domain in physical space to a simple (i.e. rectangular in 2D) flow domain in computation space. The Cartesian coordinate system *xi* in the physical domain is replaced by a curvilinear coordinate system ξi such that boundaries of the flow domain correspond to surface ξi = constant. The equations are then discretised with respect to the computational space coordinates. Boundary conditions can then be implemented naturally in the rectangular computational domain. A multi-block method is employed to further extend the geometric capabilities of the turbulent combustion code. The whole physical domain can be divided into several blocks according to the boundary types of physical domain, so that each border of a block must be of the same boundary type. The SIMPLE-like algorithm [1] is employed to solve the coupling between the velocity field and pressure. The collocated grid approach as proposed by Rhie and Chow [2] is chosen in the development of this code. The coupling algorithm suggested by Lai [3] for Reynolds stress and velocity coupling is implemented for the second order Reynolds stress model.

The full approximation scheme (FAS) of the multigrid method is employed to accelerate the convergence processes. The code is parallelised with MPI with the domain decomposition techniques. Each block must be allocated in one processor, while one processor may contain more than one blocks. Large blocks may be divided into small blocks so that a load balance can be achieved easily. The scalability of the code is examined on an IBM SMP4 machine for a case of 2000x600 grid points. The relative speedups achieved on the hardware platform are shown in Fig. 1. The speedup is based on the 4 processors.

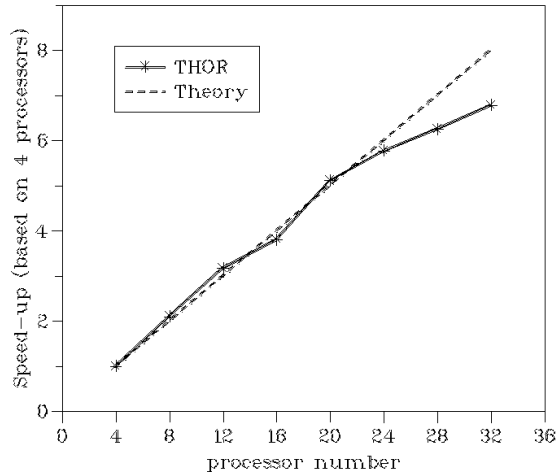

Figure 1. Observed speedups on IBM SP2

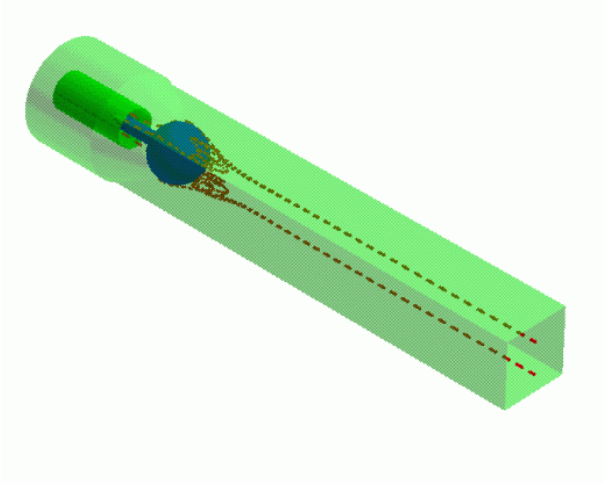

Figure 2. Flow pattern behind a sphere in a concentric capillary.

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Shown in Fig. 2 is the computed flow pattern behind a sphere in a concenric capillary used as a continues rapid mixer.

One of the significant challenges in modelling microflows is being able to handle geomertries with very large aspect ratios. As a typical example, a device could be several millimetres long but the width and depth would be 10-20 microns. This leads to aspects ratios of several thousand to one and making the use of parallel computers very attractive. Recently, Daresbury Laboratory has taken delivery of Europe's largest research facility and is known as HPC(X). The system comprises 40 IBM nodes and each node hold 32 p690 processors. The peak performance of the system is greater than 6.5Tflop/s and the machine is currently (November 2002) ranked 9th in the world. The final paper will present results from the new supercomputer in the modelling of microfluid MEMS devices.

References

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