IOWA STATE UNIVERSITY

The report from Iowa State University for the period follows.

CFD INVESTIGATION OF SLURRY BUBBLE COLUMN HYDRODYNAMICS

Fifth Quarterly Report

Reporting Period: October 1 – December 31, 2000)

Highlights

- Determined the domain size necessary to represent all the flow scales in a gas-liquid bubble column at high superficial gas velocity.
- Ported CFDLIB and conducted scaleup studies on the INTEL LINUX cluster at the Scalable Computing Laboratory, Ames Laboratory.
- Ported the parallel version of CFDLIB code to the SGi Origin 2000 at the ISU high-performance computing facility.
- Ran simulations using periodic boundary conditions for the largest domain size in order to study the hydrodynamics of a wide-diameter gas-liquid bubble column.

Summary of Progress

First, air-water bubble column simulations were performed for different grid sizes and domain sizes. An analysis of the spectra for these simulations led to the determination of the minimum domain size needed to represent all significant flow structures within the column width. Currently we are conducting simulations for a 256-cm wide column with different grid sizes.

All of our earlier simulations utilized the sequential version of CFDLIB code. At this time we have implemented a parallel version of the code, investigated periodic boundary conditions, and performed scaleup studies. The parallel version of the code cannot as yet handle periodic boundary conditions on distributed memory (cluster) computers. We are working with consultants at the ISU high-performance computing center to modify the code to correct this problem.

We plan to acquire an Alpha cluster machine for our research group during the first or second quarter of 2001. As a means of preparation, scaleup studies on the Ames Laboratory Intel Cluster were performed for three-dimensional simulations. The dimensions of the bubble column were chosen as the largest problem that can be solved using one node of the cluster. This smaller problem does not show any increase in speed of solution with a higher number of processors. Similar studies will be performed on the Ames Laboratory Alpha Cluster using the periodic boundary condition code after it has been modified for parallel machines.

Simulation Results

This section summarizes the simulation results obtained during the fourth quarter of 2000 for a two-dimensional air-water bubble column. In all cases, the air was introduced uniformly into the bottom of the column with a superficial air inlet velocity of 12 cm/sec. Grid and domain sizes for each case are listed in Table 1. The simulations were allowed to attain a statistical steady state before data were collected for time averaging.

Table 1 Description of Grid Size and Domain Size for Different Simulation Cases

Simulation case	Grid size (cm X cm)	Domain size (width X height)	Simulation time for calculation of time-averaged quantities (seconds)
1	1 X 1	**64 X 128**	50
2	2 X 2	64 X 128	72
3	2 X 2	128 X 128	150
4	4 X 4	**128 X 128**	20
5	2 X 2	**256 X 256**	20

Figure 1.1 illustrates the profile of kinetic energy of the water phase with respect to time for three different domain sizes. As shown in this figure, the largest domain size (256 X 256) displays a maximum of approximately 4500 cm^2/sec^2 at approximately 20 seconds. (The computational cost of running this simulation on a single-processor machine prohibited us from continuing the calculation beyond 20 secs.) The 128X128 domain exhibits a maximum of nearly 5000 cm^2/sec^2 at a time of 100 seconds. However, statistically its behavior is very similar to that of the largest domain. For the smallest domain size (64 X 128), the kinetic energy tended to increase with time throughout the 150-second period observed, and exhibited much smaller fluctuations. The value at the end of the run was very similar to the other cases. The lower fluctuation levels were undoubtedly due to low-pass filtering of the velocity fields by the “coarse” computational grid.

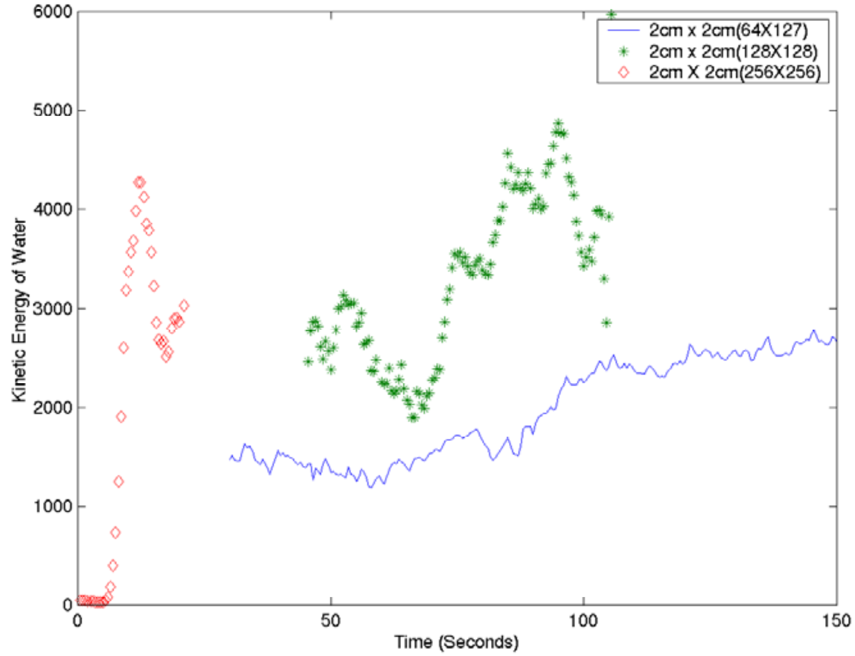

Figure 1.1 Sample Kinetic Energy (cm^2/sec^2) Time Series in Water Phase for Three Different Domain Sizes

Figures 1.2 and 1.3 show the spectra of water velocity components for four different cases. The abrupt decrease at the Nyquist frequency [defined as 1/(2*sampling interval)] signifies that the (molecular) viscous dissipation term of the multi-component momentum equations are not resolved for these flows. This cut-off implies that we are essentially neglecting the viscous dissipation term. The simulations are then essentially *inviscid* two-phase flow (with grid spacing greater than or equal to 1 cm) and rely on the low-pass filtering property of the grid to dissipate energy (i.e., crude LES). Since most CFD studies that have appeared in the literature have used a grid size on the order of 1 cm for the air-water system, these must also suffer from under-resolution. It can also be observed in Figure 1.2 that the total energy of the spectra increases with increasing resolution. Note also in Figure 1.3 that the vertical velocity component (v) is slightly more energetic than the horizontal component, as would be expected due to the vertical drag force. Similar (and perhaps even stronger) anisotropy has been observed in the bubble-column experiments of Zenit, et. al. (2000). We plan to explore this question further by performing simulations of the Zenit experiment in the coming year.

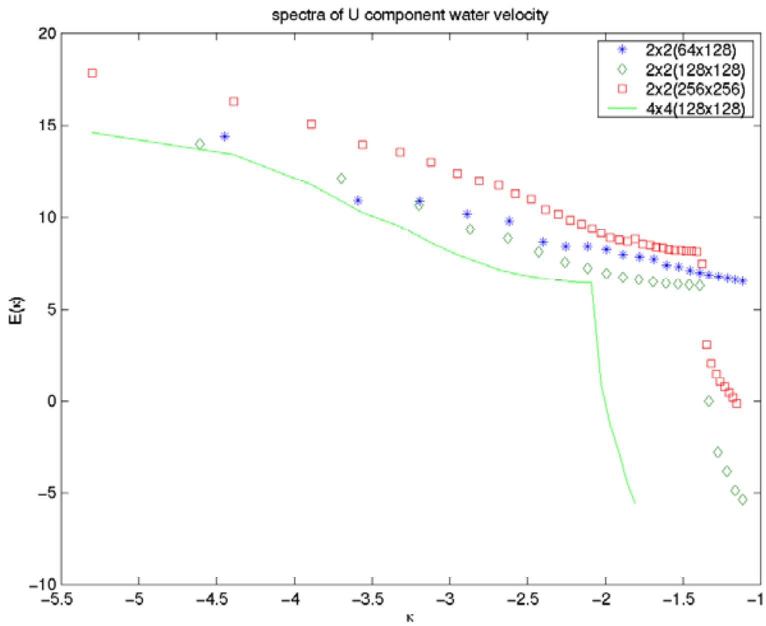

Figure 1.2 Spectra of U Component of Water Velocity for Four Different Cases

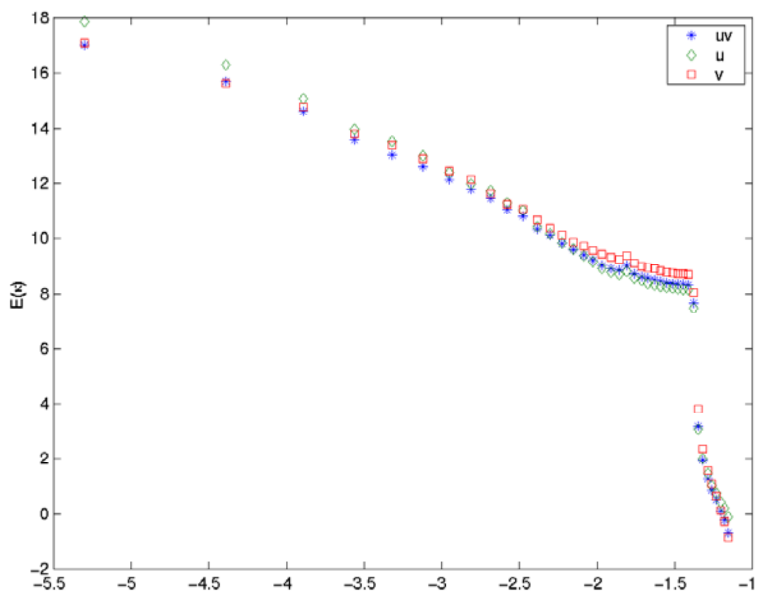

Figure 1.3 Spectra of u, v and Cross Term of Water-Phase Velocity for Case 5 LINUX Cluster Scaleup Study

The computational cost associated with three-dimensional, high-resolution simulations has led us to port CFDLIB to parallel hardware. In order to test the computational gains that are achievable using multiple processors, a scaleup study was performed on the Ames Laboratory INTEL cluster. For this study, the following column parameters were used:

Length = 50 cm Height = 160 cm

Width = 50 cm Grid Spacing = 1 cm

In addition, it was assumed that air was introduced uniformly to the column at a rate of 8 cm/sec. The average time taken per iteration is shown in Table 2 and Figure 2.1.

Table 2 Average Time per Iteration taken by CFDLIB on INTEL LINUX Cluster for Different Numbers of Processors

Number of Processors Used	Average time per iteration (in minutes)
1	2.83
3	2.07
4	1.92
5	1.45
8	1.02

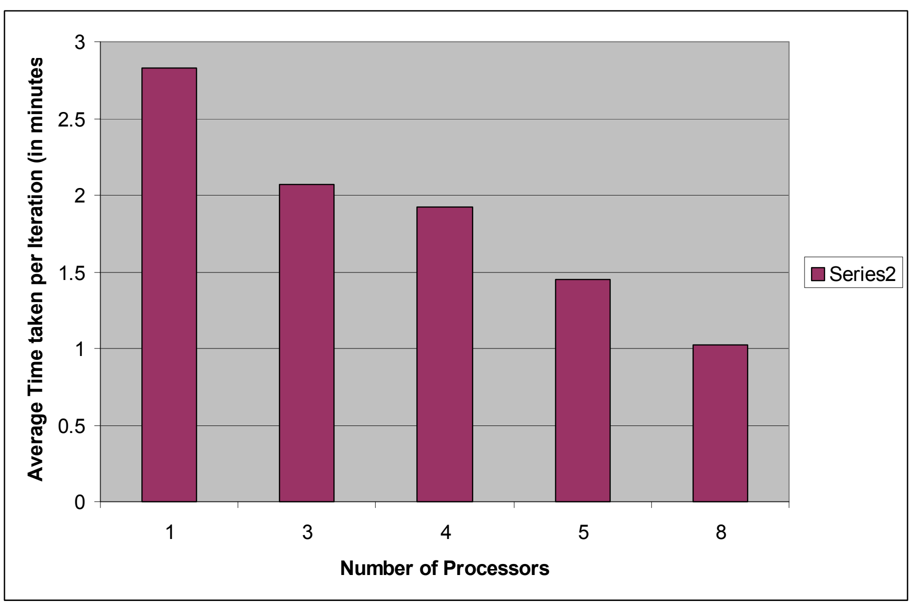

Figure 2.1 Average Time (minutes) per Iteration for Various Numbers of Processors

As shown in Table 2 and Figure 2.1, using eight processors improves the speed by a factor of 2.24 over the use of a single processor, which is reasonable when compared to the ideal speed-up factor of 4. Since CFDLIB is a block-structured code, the time taken per iteration should halve on doubling the number of processors. From this study, it appears that going beyond eight processors may improve the performance, but the gains will be modest. It was also discovered in the process of running these simulations that the parallel version of the code with periodic boundary conditions yields incorrect answers. We are thus looking into the cause of this problem with the help of the consultants at the ISU High-Performance Computing group. The next step in the parallelization study will be to port the code to the Ames Laboratory Alpha cluster. The single-processor speed of the Alpha is 4-5 times faster than the SGi Origin. This increase in performance should yield better scaleup characteristics on the Alpha cluster than the Intel cluster for large problems. We plan to purchase an Alpha cluster for our research group in the first quarter of 2001.

Future Work

Iowa State will next study free-slip boundary conditions versus periodic boundary conditions to determine whether or not free-slip boundary conditions could be a suitable alternative. Also, CFDLIB will be used to simulate conditions described in Zenit et al.

References

Zenit, R., D.L. Koch, and A.S. Sangani, Measurements of the average properties of a suspension of bubbles rising in a vertical channel, *J. Fluid Mech.* Vol. 420, pp.1-36 (2000).