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CLUSTER: "Studies in Macromolecular Behavior in a Microgravity Environment"

The Role of Protein Oligomers in Protein Crystallization (W. Wilson, Mississippi State University)
High performance size exclusion chromatography (HPSEC) was used to obtain the monomer fraction for thirteen proteins varying in molecular weight (M) from 13,700 to 680,000 g mol $^{-1}$. Dynamic laser scattering (DLS) was used to measure the translational diffusion coefficients (D) and diffusion virial coefficients of each protein in 20 mM sodium phosphate buffers, ph=7.5 with 0.1 M NaCl. A calibration curve was constructed relating log M and log D which showed a high degree of linear correlation. The empirical relationship obtained from this data was $D=4.38 \times 10^{-5} M^{-0.379}$ cm ^{2}/sec. This relationship can be very useful for estimating the molecular weight of aggregates that are often present in protein solutions used for crystallization experiments.

Phase Separation Phenomena in Microgravity (L. Mathias, The University of Southern Mississippi)
The jump start fund provided for a one-year initiation project which was used in two efforts. The first involved collaboration with John Pojman in Chemistry in the area of traveling front polymerizations. This project resulted in one rocket flight (see his section of the report) and one KC135 joint publication. The second area focused on phase separation phenomena in microgravity. This component involved a "piggy back" experiment flown with collaborators at the University of Alabama-Huntsville and Marshall Space Flight Center. The ten experimental cells that we were allowed to incorporate into their reactors involved several key experiments in which phase separation during polymerization would be locked by the polymerization process. Unfortunately, two of three ovens were damaged during the launch and recovery process, and only one reactor performed successfully. We retrieved four cells from this reactor, all which showed excellent conversion and polymerize materials within locked-in domains. Because of the failure of the other reactors, however, we were unable to do the comparison of concentrations and rates of reaction necessary for complete interpretation of the results. It should be noted that the four cells clearly showed differences with respect to earth-based polymerization, although these differences have not been quantitated to date. We are developing SEM and TEM capability which will allow us detailed analysis of the domain sizes and regularities.

Traveling Front Polymerizations (J. Pojman, The University of Southern Mississippi)
With "jump start" funds, we constructed a reactor to fly on the Conquest I sounding rocket. The Conquest I rocket took our experiment to 178 miles above the earth for six minutes of weightlessness after launching from White Sands Missile Range in New Mexico on April 3, 1996. We tested how fronts of n-butyl acrylate polymerization propagate when bubbles are present (bubbles are large and occur periodically) and how surface-tension induced convection can affect fronts. By comparing the properties of samples produced in microgravity to ground-based ones, we determined that silica gel added in ground-based experiments to suppress convection does not significantly affect the product's molecular weight distribution. Using the same reactor, we flew KC-135 flights in early December. Analysis of those results is still underway.

Investigating Mechanisms Affecting Phase Transition Response and Changes in Thermal Transport Properties in ER-Fluids under Normal and Microgravity Conditions (S. Sinha, The University of Mississippi)
Electro-rheological fluids or ER fluids are suspensions of small electrically polarizable solid particles in a dielectric liquid. When subjected to a strong electric field, the solid particles in an ER fluid form closely connected chains, giving the appearance of the fluid transforming into a solid. The change is completely reversible and fast. The primary focus of this study was to determine electric field induced changes in the effective thermal conductivity and heat capacity of ER fluids. Experiments were conducted with two commonly available mixtures: (1) corn starch and peanut oil, and (2) cellulose and silicone oil. The mixtures were enclosed in a 62.5 mm square 5-mm deep horizontal test cell. The cell was

heated from below and cooled from above and insulated around the edges. The heat transfer rates to and from the cell were monitored along with temperatures of the hot and cold sides. The electric field was applied vertically with a maximum intensity of 12-kV/cm. Experiments revealed that the effective thermal capacity of the cell increased with voltage for mixture (1) by about 10% while a decrease followed by an increase was observed for mixture (2). The effective heat capacity of the cell dropped by 50% for mixture (1) with the field while a 120% increase was observed for (2). The changes can be attributed to attenuation of natural convection in the liquid phase and an increase in conduction along the particle chains.

CLUSTER: "Computational/Parallel Processing Studies"

Several related topics in numerical algorithm design, computational analysis, and computer science have been examined as a result of NASA seedfunding of the Mississippi Research Consortium's efforts. These efforts included two projects addressing the development of numerical models for convection/diffusion problems associated with the analysis of multi-phase and chemically reacting flows occurring under extreme dynamic conditions, and a project investigating the solution of partial differential equations using wavelets. The projects focused on enhancing competitiveness and the primary effort was to develop research models and algorithms suitable for efficiently solving these problems, especially in regard to extending these efforts to parallel computer architectures.

Flows in Local Chemical Equilibrium (P. Cinella, Mississippi State University)
The project has resulted into the parallelization of a three-dimensional flow solver, which has been used for the numerical simulation of problems involving arbitrary mixtures of thermally perfect gases. Local chemical equilibrium is assumed to exist at every point in the flowfield, which allows for an inexpensive inclusion of high-temperature, high-velocity effects ("real gas" effects) in the physical modeling. The solution procedure is by no means limited to external flows in air, and has been applied to fuel/air and weakly ionized plasma mixtures as well.

A "Black Box" solver for the local equilibrium composition of a gas mixture of known density and internal energy is coupled with the flow solver, which is based upon an approximate Riemann solver of the Roe type. A preliminary study of the parallel performance of the code for single-block, inviscid test cases was conducted, then more realistic viscous multi-block test cases were examined. The code has been ported to the Cray T3D parallel computer. Test runs indicate significant reductions in execution time.

References

1. Wei, S., Zhu, J., Cox, C.F., and Cinnella, P., "On the Parallelization of a Three-Dimensional "Real Gas" Flow Solver," Paper No. 95-0571, AIAA 33rd Aerospace Sciences Meeting., 1995.

2. Carino, R. L., Zhu, J., Cox, C.F., and Cinnella, P., "Parallel Performance of a Three-Dimensional Viscous Multi-Block "Real Gas" Flow Solver," *First International Conference on Nonlinear Problems in Aviation and Aerospace,* Daytona Beach, Florida, May 1996.

A Computational Method for Solving Very Large Problems (R. Gordon, The University of Mississippi)
The work conducted by Richard Gordon and his graduate students at the University of Mississippi concerned the use of wavelet-like basis functions in the finite element solution of ordinary and partial differential equations. These basis functions are of interest because when they are used in conjunction with simple diagonal preconditioning, the condition number of the resulting finite element matrix is bounded by a constant as the number of basis functions is increased, whereas, when the traditional finite element basis functions are used, the condition number increases without bound under the same circumstances. This boundedness of the condition number leads to rapid convergence of iterative solution techniques and the avoidance of numerical instabilities.

The algorithm for generating the wavelet-like basis functions was partially parallelized at the start of the project. But the eigenanalysis part was still unparallelized. One of the main goals was to make this part of the code more efficient, either through parallelization or the development of an alternative procedure. Lee Harrison, a graduate student working under Dr. Gordon's supervision, found a method for developing alternative wavelet-like basis functions that, in every

case studied so far (in both the 1-D and 2-D cases), have lead to even lower condition numbers than those obtained with the original wavelet-like basis functions. Furthermore, these alternative wavelet-like basis functions can be generated in a small fraction of the time required for the original wavelet-like basis functions. Now, work is proceeding on the parallelization of the finite element code that utilizes these basis functions. In both the 1-D and 2-D cases, the algorithm has been parallelized; all that remains is the actual writing and testing of the parallel code. The serial code has been written and extensively tested.

Modeling of Cavitating Flows (J. Kolibal, The University of Southern Mississippi)
The simulation of cavitating flows involving large sheet cavities is developed using an adaptive interface tracking algorithm which is used to adjust the solutions for the bulk flow field obtained by using an unstructured mesh based finite volume method. The front tracking is accomplished using the total momentum associated with the flow field impacting on the bubble and it takes into account the surface tension of the bubble. While Chorin's method, which is used to compute the flow field is expectable slow to converge, it is workable and provides a solution mechanism which can take advantage of the large number of standard techniques which have been developed to accelerate the convergence of hyperbolic, compressible flow problems based on similar finite volume techniques.

Bubble tracking using an explicit free boundary formulation is accomplished using an update of the bubble surface (outer iteration) associated with each solution of the steady state flow field (the inner iterations used to determine the surrounding flow field). The bubble surface is traced using a search algorithm based on detecting the inception point with the update of the bubble boundary taking account of the pressure, velocity, and surface tension. Care is taken to define this interface boundary with regard to constructing locally a new grid aligned with the interface. The solution algorithm is begun with no bubble present in the flow field.

A simple algebraic scheme suffices to regrid the flow field in the vicinity of the new interface after the grid vertices along the free surface are adjusted to maintain a smooth transition and spacing and the grid is refined and re-triangulated to produce the updated, unstructured grid with the new cavity surface being incorporated as a slip boundary and a new steady-state flow field is computed using these boundary conditions. This procedure is continued iteratively until the bubble ceases to change shape, i.e., convergence is achieved when a fixed point is found for the inner and outer iterations.

Overall, the initial results are encouraging and serve to demonstrate that it is possible to efficiently distinguish even small changes of the bubble shape, even at the trailing edge, by judiciously making use of the local mesh refinement technique. Most importantly, this can be accomplished with the need to develop arbitrary closure conditions.

Parallelizing the code on the Cray T3D at the Pittsburgh Supercomputing Center (PSC) has shown encouraging speedups which scale well with the number of processors. Parallelization has been implemented for the flow solver, however, full parallelization of the front tracking remains to be done.

Further research is needed to include more physical phenomena into the modeling of the free boundary. In particular, the lack of an energy equation in this model is a deficiency which requires attention, particularly if the modeling of the energy transfer across the interface is to be correctly accounted.