NASA CONTRACTOR REPORT

STATISTICAL DISCRETE PARTICLE SIMULATION STUDIES

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Ames Research Center
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16. Abstract

A particle simulation code was developed that is suited to Multiple Instruction Multiple Data multiprocessor computers. The resulting code is designed to be portable between a large class of multiprocessor computer architectures, including hypercubes (e.g., Intel iPSC/860), shared memory machines (e.g., CRAY, SGI, DASH), and simple uniprocessors (e.g., SUN, VAX, IBM PC). This code provides a powerful general framework that can be adapted to specific applications, such as thermochemical modeling, general 3-dimensional geometry support, or visualization support via a co-developed CPlot data reduction and visualization system.

Chemistry models developed by B. Haas were implemented and validated with comparison to continuum solutions of thermochemically relaxing gas mixtures and with experimental results from the high-speed flow about a circular cylinder.

Furthermore, the exchange of energy between translational and internal modes was modeled. New models were developed, combining greater efficiency than earlier phenomenological models such as those by Borgnakke and Larsen. They offer greater physical detail by addressing vibrational energy as a discretely distributed quantity.

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INTRODUCTION

This is a final report on work carried out since January 1st 1990 in the Aerothermodynamics branch and NASA Ames research center. In a 1989 Ph.D. thesis by Dr. J. McDonald, algorithms for a direct particle simulation method were reformulated to permit efficient vectorization. Speedups of approximately 100 times over conventional methods at that time were achieved. These advances demonstrated the advantages of using algorithms specifically tailored to a given high performance computer architecture in computationally intensive scientific applications. This early research resulted in a computer code that could address multiple specie gases in three-dimensional flow fields.

Since that time, work has continued on both computational and physical aspects of particle simulation techniques. A number of papers and presentations were prepared. In this report, work is categorized into three distinct areas, namely, computational advances in utilizing multiprocessor computers, chemistry validation efforts, and physical modelling advances.

MULTIPROCESSOR IMPLEMENTATION

A large effort during this study has gone to developing a particle simulation code that is suited to Multiple Instruction Multiple Data (MIMD) multiprocessor computers. The resulting code is designed to be portable between a large class of multiprocessor computer architectures including hypercubes (eg. Intel iPSC/860), shared memory machines (eg. Cray, SGI, DASH), and simple uniprocessors (eg. Sun, VAX, IBM PC). Portability

has already been demonstrated on several different machines. This code provides a powerful general framework that may be modified for specific applications of interest by other researchers. Included are thermo-chemical modelling, general three-dimensional geometry support, and visualization support via the co-developed CPlot data reduction and visualization system (by Dr. J. McDonald and Mr. M. Fallavollita). It is hoped that this software will see continued development and application to problems in rarefied gas dynamics in coming years.

This work was reported at the AIAA Thermophysics Conference in Hawaii in June 1991 and that paper is included as appendix A.

CHEMISTRY VALIDATION

The implementation of the chemistry models developed by Dr. Brian Haas in his thesis have been extensively validated with comparison to continuum solutions of thermochemically relaxing gas mixtures and with experimental results from the high speed flow about a circular cylinder. This work was presented at the AIAA thermophysics conference in Hawaii. The accompanying paper is included as appendix B.

PHYSICAL MODELLING

Of continued interest in the field of particle simulation is the modelling of collision mechanics. Specifically, the exchange of energy between translational and internal modes is of ongoing interest. Phenomenological models such as those by Borgnakke and Larsen have been the mainstay in

particle simulation methods since their inception. This is due primarily to the computational efficiency of such models and the lack of understanding of any further detail. New models have been developed here, that combine even greater efficiency than earlier phenomenological models while at the same time offering greater physical detail by addressing vibrational energy as a discretely distributed quantity. This work is presented in Appendix C in the form of a Journal article as submitted to the Journal of Computational Physics.

Work is also underway to determine if experimentally know gas mixture viscosity data can be captured in a more natural way than is currently done. Typically, one interaction potential is utilized for all collision classes between the var ecies in a multi-specie simulation. This single potential is determine om experimental viscosity data for a gas mixture at a reference condition common to both experiment and the simulation. Recognizing that this can adversely impact specie diffusion as the gas composition is altered through mass diffusion or chemistry, it is felt that a more physical approach is desirable. Work is being done to show that this is an important omission from current approaches and that by using different interaction potentials for each collision class, mixture viscosity behavior can be directly obtained. Collision interaction potentials and cross sections between like molecules are easily characterized in the simulation using experimentally derived single specie viscosity data. Unknown cross potentials and collision cross sections are then determined through parametric studies

comparing simulation determined mixture viscosities with experimentally obtained mixture viscosities. This work will be continued by Dr. Iain Boyd