GRANT
IN-39-CR
194055
11P

PROGRESS REPORT

NASA PROPOSAL NAG3-1410
C.U. # 153-6505

L. SANI
DEPARTMENT OF CHEMICAL ENGINEERING
CENTER FOR LOW GRAVITY FLUID MECHANICS
AND TRANSPORT PHENOMENA
UNIVERSITY OF COLORADO

PROGRESS REPORT

Modeling and New Equipment Definition for the Vibration Isolation Box Equipment System

R.L. Sani
Department of Chemical Engineering
University of Colorado
Boulder, CO 80309-0424

Our MSAD-funded research project is to provide numerical modeling support for the VIBES (Vibration Isolation Box Experiment System) which is an IML2 flight experiment being built by the Japanese research team of Dr. H. Azuma of the Japanese National Aerospace Laboratory. During this reporting period, the following have been accomplished:

1. **A Semi-Consistent Mass Finite Element Projection Algorithm For 2D And 3D Boussinesq Flows Has Been Implemented On Sun, HP And Cray Platforms.**

   a. The algorithm has better phase speed accuracy than similar finite difference or lumped mass finite element algorithms, an attribute which is essential for addressing realistic g-jitter effects as well as convectively-dominated transient systems.

2. **The Projection Algorithm Has Been Benchmarked Against Solutions Generated Via The Commercial Code FIDAP.**

   a. The algorithm appears to be accurate as well as computationally efficient.

3. **Optimization And Potential Parallelization Studies Are Underway.**

   a. Our implementation to date has focused on execution of the basic algorithm with at most a concern for vectorization.

4. **The Initial Time-varying Gravity Boussinesq Flow Simulation Is Being Set-up.**

   a. The mesh is being designed and the input file is being generated. Some preliminary "small mesh" cases will be attempted on our HP9000/735 while our request to MSAD for supercomputing resources is being addressed.

5. **The Japanese Research Team For VIBES Was Visited, The Current Set-up And Status Of The Physical Experiment Obtained And Ongoing E-Mail Communication Link Established.**

REQUEST FOR NASA SCIENTIFIC COMPUTING RESOURCES

Robert L. Sani
University of Colorado
Department of Chemical Engineering
Boulder, Colorado 80309-0424

Our MSAD-funded research is to provide numerical modeling support for the VIBES (Vibration Isolation Box Experiment System) which is an IML2 flight experiment being built by the Japanese research team of Dr. H. Azuma of the Japanese National Aerospace Laboratory. This request of scientific computing resources is made to support flow and transport modeling for ground base pre-flight experimental design and validation experiments, post-flight data analysis as well as an assessment of the potential of using data and hardware for future flight experiments. In order to accomplish these goals, the transient Navier-Stokes and/or Boussinesq equations in three space dimensions including a complicated time varying gravitational body force must be solved. A new semi-consistent mass projection algorithm has been developed to generate time-accurate solutions. This algorithm has better phase speed accuracy than similar finite difference or lumped mass finite element algorithms and appears to be very efficient computationally, both necessary attributes for addressing realistic g-jitter effects as well as transient systems dominated by convective transport. (A brief description of the project and algorithm are in Appendix 1.) The development and preliminary benchmarking of the algorithm has been done on our HP9000 workstation, but access to a supercomputer platform is essential to support the very large 3D transient simulations especially necessary in the post-flight data assessment and in new experiment assessment; such simulations even when theoretically possible on a workstation are practically intractable because of the amount of computational time required. The algorithm has been designed such that the porting to a supercomputer such as a CRAY Y-MP will be very easy as will be the efficient use of its vectorization capability. Parallelization is an issue which we are currently addressing; the possibility of utilizing the efficient NASA parallel-vector direct solution algorithm due to Storaasli et. al. is already incorporated. Other parallelization via iterative solvers will eventually be addressed but only aggressively at a later date because of the time-line constraint of our MSAD project. The algorithm on the CRAY Y-MP is dynamically dimensioned and for the types of 3D meshes which seem to be appropriate for production runs, we will require approximately 64 megawords and an estimated 100 hours of computing time for algorithm porting enhancement, optimization and the production runs. The latter is difficult to estimate because of our desire to use an actual filtered g-jitter signature in the post-flight stage of the project.

APPENDIX 1

PROJECT DESCRIPTION

A. Introduction

In a terrestrial environment, natural convection and concomitantly the heat and mass transport processes intimately associated with it can sometimes have a deleterious effect on a process; for example, in materials processing where it, in conjunction with other effects such as walls or moving interfaces, can lead to radial segregation and dopant striations in the product material. In view of this, there has been a desire to use the space environment in order to reduce natural convection and other gravitational effects as well as make containerless processing more viable. In many cases, the ensuing dominance of surface-tension-driven flows in a micro-gravity environment has led to a significant number of similar as well as new problems. To further complicate matters, the micro-gravity environment available is not quiescent but is subjected to significant background vibrations generated by aerodynamic, structural and machinery vibrations, crew motion, etc. Such g-jitter can be relatively random in orientation and attain significant magnitudes such as $10^{-2}g_0$ (g_0 = earth g) experienced during thruster firing on the D1 mission to the less significant $10^{-5}g_0$ experienced on the SPAR-X free flyer. There is a growing list of observations and data analyses that demonstrate the existence of significant g-jitter episodes and the potential for having very deleterious effects on many proposed flight experiments as well as negate the potential of a micro-gravity environment. In addition, numerical and analytical modeling studies suggest that g-jitter effects could seriously affect many micro-gravity experiments as well as possibly space commercialization ventures, especially in the materials science area. An interesting potential solution to this problem in the micro-g environment available on shuttle flights or planned on Space Station Freedom is the use of vibration isolation for the experiments and processes which require it. The assessment of such an apparatus is one of the main thrusts of the research proposed herein.

The experiment VIBES (Vibration Isolation Box Experiment System) is an IML2 flight experiment being designed by a Japanese research team under the direction of Dr. Hisao Azuma of the Japanese National Aerospace Laboratory. Its basic objective is to assess the performance of a vibration-isolation device in conjunction with typical micro-g fluids experiments. The device has been specifically designed for the low frequency range which appears to be most deleterious to many micro-g experiments, especially those material science experiments dealing with coupled flow and transport processes and could provide a relatively simple and economical means of dealing with such g-jitter problems. The IML2 flight experiment will contain two experimental units:

1. Convection Diffusion Unit (CDU)
2. Thermal-Driven Flow Unit (TDFU)

The CDU experiment is the one of interest herein; the main objectives of this experiment are to observe natural convection and diffusive transport in a micro-g environment and to observe the effect of a g-jitter with and without the vibration isolation due to the vibration isolation box. The semi-consistent mass projection method algorithm summarized hereafter has been inplemented to provide flow and transport modeling capability for ground-based experiment

design and validation and post-flight data analysis as well as an assessment of the potential of using the data and hardware for a future flight experiment. It is designed to solve the transient Navier-Stokes, or Boussinesq equations in two or three space dimensions. Time accurate solutions are obtained by using a semi-consistent mass projection algorithm [Gresho (1990)]. Theoretically this algorithm has better phase speed accuracy than similar finite difference or lumped mass finite element algorithms, a property which is very desirable for the g-jitter simulations being addressed as well as other convective transport dominated systems.

CONTINUUM MODEL

In terms of the Boussinesq equations, the appropriate continuum equations for the velocity (u), temperature (T), and kinematic pressure (P) are:

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = -\nabla P + v \nabla^2 u + f \quad , \qquad \text{in } \Omega \tag{1a}$$

$$\nabla \cdot u = 0 \quad , \qquad \text{in } \overline{\Omega} \tag{1b}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + u \cdot \nabla T \right) = k \nabla^2 T + q \quad , \qquad \text{in } \Omega \tag{1c}$$

The vector f represents body forces, for example, buoyancy,

$$f_{\text{buoyancy}} = -\frac{(\rho_o - \rho(T))}{\rho_o} g$$

where g is the gravitational vector which in our case will be time-dependent, v is the kinematic viscosity, ρ (ρ_o) is the density (reference density), C_p is the specific heat and k is the thermal conductivity. If the boundary of Ω is designated by $\partial \Omega = \Gamma_1 \oplus \Gamma_2$, then typical appropriate boundary conditions are specified velocity and temperature (Dirichlet):

$$u = w \quad , \qquad T = T_B \tag{1d}$$

on Γ_1 and 'pseudo traction' and specified flux conditions (Neumann)

$$-P + v \frac{\partial u_n}{\partial n} = F_n \quad \text{and} \quad v \frac{\partial u_\tau}{\partial \tau} = F_\tau \tag{1e}$$

$$k \frac{\partial T}{\partial n} = h(T - T_a) + q$$

on Γ_2 . Here $\mathbf{n}$ represents the outward normal direction, $u_n = \mathbf{u} \cdot \mathbf{n}$ is the normal component of velocity, τ represents the corresponding tangential direction, $u_\tau = \mathbf{u} \cdot \tau$ is the tangential component of velocity and F_n and F_τ are the normal and tangential components of the specified boundary traction. (All combinations of BC's (Equations 1c and 1d) are possible in three-dimensional simulations))

To complete the problem specification, initial conditions must be specified:

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}) \tag{1f}$$

$$T(\mathbf{x},0) = T_0(\mathbf{x})$$

The initial velocity field is required to satisfy the following conditions:

$$\mathbf{n} \cdot \mathbf{u}_o = \mathbf{n} \cdot \mathbf{w}(\mathbf{x},0) \quad \text{on } \Gamma_1 \quad \text{and} \tag{1g}$$

$$\nabla \cdot \mathbf{u}_0 = 0 \quad \text{in } \Omega \tag{1h}$$

in order that a solution exists [Gresho and Sani (1987)]. Should $\Gamma_1 \equiv \partial \Omega$, global mass conservation

$$\int_{\partial \Omega} \mathbf{n} \cdot \mathbf{w}(\mathbf{x},\, t) = 0 \tag{1i}$$

is an additional solvability constraint.

The continuum version of the projection technique is a finite element discretization (with some modifications) of those proposed by Van Kan (1986) and Bell and Marcus (1990) as described in Gresho (1990). The algorithm is:

0)   Given $\mathbf{u}_0$ with $\nabla \cdot \mathbf{u}_0 = 0$ and P_0 ,

1)   Solve for $\bar{\mathbf{u}}$ and $\bar{T}$, with $\bar{\mathbf{u}}_0 = \mathbf{u}_0$ and $\bar{T} = T_0$ at $t=0$ from

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \bar{\mathbf{u}} \cdot \nabla \bar{\mathbf{u}} - \nu \nabla^2 \bar{\mathbf{u}} = \mathbf{f} - \nabla P_0 , \quad \text{in } \Omega \tag{2a}$$

$$\rho C_p (\frac{\partial \bar{T}}{\partial t} + \bar{\mathbf{u}} \cdot \nabla \bar{T}) = k \nabla^2 \bar{T} + q , \quad \text{in } \Omega \tag{2b}$$

$$\bar{\mathbf{u}} = \mathbf{w} \quad \text{and} \quad \bar{T} = T_B , \quad \text{on } \Gamma_1 , \tag{2c}$$

$$v\frac{\partial \tilde{u}_n}{\partial n} = F_n(t) + P_0 \quad \text{and} \quad v\frac{\partial \tilde{u}_\tau}{\partial \tau} = F_\tau(t) \quad , \quad \text{on } \Gamma_2 \tag{2d}$$

$$k\frac{\partial \tilde{T}}{\partial n} = h(\tilde{T} - T_a) + q$$

for $0 < t < t_1$, where $[0, t_1]$ is the time span between two projections. Since the intermediate velocity $\tilde{u}$ is not divergence free, solve the following least squares problem at projection time T:
Extremize:

$$G(\mathbf{v}, \varphi) \equiv \int \frac{1}{2}(\mathbf{v} - \tilde{u})^T (\mathbf{v} - \tilde{u}) - \varphi^T \nabla \cdot \mathbf{v} \tag{3a}$$

Subject to appropriate boundary conditions;

i.e., set the first variation equal to zero to obtain (after an integration by parts):

$$(\mathbf{v} - \tilde{u}) + \nabla\varphi = 0 \quad \text{and} \tag{3b}$$

$$\nabla \cdot \mathbf{v} = 0 \quad \text{in } \Omega \,, \tag{3c}$$

with $\mathbf{n} \cdot \mathbf{v} = \mathbf{n} \cdot \tilde{u}$ on Γ_1 and $\varphi = -\frac{t_1}{2}[F_n(t_1) + P_0]$ on Γ_2.

or in practice,

2)   Solve for φ from

$$\nabla^2\varphi = \nabla \cdot \tilde{u} \quad \text{in } \Omega \,, \tag{3d}$$

subject to

$$\frac{\partial \varphi}{\partial n} = 0 \quad \text{on } \Gamma_1 \quad \text{and} \tag{3e}$$

$$\varphi = -\frac{t_1}{2}[F_n(t_1) + P_0] \quad \text{on } \Gamma_2. \tag{3f}$$

3)   compute $\mathbf{v} = \tilde{u}(T) - \nabla\varphi \quad \text{in } \Omega$ \hfill (4)

4)   Estimate a new pressure: $P(T) = P_0 + 2\varphi / t_1 \quad \text{in } \Omega$ \hfill (5)

5) Report v and P; then set $t=0$, $P_0 = P(t_1)$, $u_0 = v$ in Ω and go to step 1.

DISCRETIZATION

The continuum formulation is discretized in space via a Galerkin finite element method. For efficiency, the finite element representation is restricted to four node (in 2D) or 8 node (in 3D) elements for velocity and temperature and a piecewise constant pressure approximation. Even though these element combinations are degenerate, i.e., the velocity-pressure basis function combination possesses a null space, it is easily accommodated [Sani, Gresho, Lee and Griffiths (1981)]. The use of a basic Galerkin finite element discretization technique automatically accommodates complex spatial domains and the complex boundary conditions on Γ_2 which are *natural* boundary conditions in the weak Galerkin finite element formulation.

The continuous-in-time Galerkin finite element spatial discretization is then temporally discretized using the Leismann scheme. [Leismann and Frind (1989)] which is second-order accurate and unconditionally stable in the form implemented but a bit dissipative or the Gresho and Chan (1990) scheme which is similar but less dissipative. The discrete system for each time step of the Leismann scheme is:

$$(\frac{1}{\Delta t}M + D + \frac{1}{2}D_{BTD})_i \tilde{u}_i = (\frac{1}{\Delta t}M - V - \frac{1}{2}D_{BTD})_i u_{oi} - MM_L^{-1}(C_i P_o - f_{oi}(T)) \quad , \quad i = 1, 2, 3 \qquad (6a)$$

$$(\frac{1}{\Delta t}M + D + \frac{1}{2}D_{BTD})T = (\frac{1}{\Delta t}M - V - \frac{1}{2}D_{BTD})T_o + q_o \quad , \qquad (6b)$$

and

$$(C^T M_L^{-1} C)\varphi = C^T \tilde{u} \qquad (7)$$

for φ needed to project the intermediate velocity $\tilde{u}$ to the weakly divergence free subspace, i.e., the final, weakly divergence free velocity u after a time step is

$$u = \tilde{u} - M_L^{-1} C\varphi \qquad (8)$$

and the corresponding pressure field is:

$$P = P_0 + 2\varphi / \Delta t \qquad (9)$$

The various element matrices M, D, D_{BTD} V and M_L are defined in Gresho and Chan (1990). The two most noteworthy features of this discretization are:

1. The consistent mass matrix **M** is used in the conservation of momentum and energy equations (6a,b) but lumped mass matrix $\mathbf{M_L}$ in the solenoidal velocity constraint equation (7).
2. The discretized system of uncoupled algebraic equations (6a, i.e. 1,2,3; 6b) are linear symmetric positive definite systems.

Feature (a) leads to phase speed accuracy while maintaining computational efficiency. Feature (b) allows the utilization of computationally efficient interative solvers such as pre- conditioned conjugate gradient solvers or, for example, the PVS-solver [Storaasli et. al.] (1990) which is a vectorized-parallelized efficient direct solution technique.

IMPLEMENTATION

The algorithm has been implemented on HP9000/735 and SUN/10 workstations and has been benchmarked against solutions to both Navier-Stokes and Boussinesq flows generated via the commercial code FIDAP [Engelman (1993)]. The current version utilizes primarily a pre-conditional conjugate gradient solver and a constant time step scheme with a variable time step version under development. The algorithm has been structured for easy vectorization and the possibility of also addressing the issue of parallelization, via the Storaasli algorithm initially and other iterative techniques eventually.

REFERENCES

1. Bell, J.B., D.L. Marcus, A Second-Order Projection Method For Variable-Density Flows, UCRL-JC-104132, LLNL, 1990.

2. Engelman, M., Fidap Users Manuals, Ver. 7, Evanston, IL (1993)

3. Gresho, P.M., On the theory of semi-implicit projection methods for viscous incompressible flow and its implementation via a finite element method that also introduces a nearly-consistent mass matrix, Part 1: Theory, *Int. J. Num. Meth. Fluids,* 11, 587-620, (1990).

4. Gresho, P.M. and S.T. Chan, On the theory of semi-implicit projection methods for viscous incompressible flow and its implementation via a finite element method that also introduces a nearly-consistent mass matrix, Part 2: Implementation, *Int. J. Num. Meth. Fluids,* 11, 621-660, (1990).

5. Leismann, H.M. and E.O. Frind, A Symmetric-Matrix Time Integration Scheme for the Efficient Solution of Advection-Dispersion Problems, Water Resources Research, Vol. 25, No. 6, pp. 275-280, (1989).

6. Sani, R.L., P.M. Gresho, R.L. Lee , and D. Griffiths, The Cause and Cure of the Spurious Pressures Generated by Certain FEM Solutions of the Incompressible Navier-Stokes Equations," Part 1 and Part 2, *Int. J. Num. Meth. Fluids,* 1: 17-43 (1981); 1: 171-204 (1981).

7. Storaasli, O.O., T. Nguyen and T.K. Agarwal, A Parallel-Vector Algorithm for Rapid Structural Analysis on High-Performance Computers, NASA Technical Memorandum 102614, Langley Research Center, Hampton, Virginia 23665-5225, (1990).

8. Van Kan, J., A Second-Order Accurate Pressure Correction Scheme for Viscous Incompressible Flow, *SIAM J. Sci. Stat. Comp.,* Vol. 7, No. 3, pp. 870-891, (1986).