

NASA GSRP 2003-2004 Progress Report: Parallel finite element techniques and adaptive mesh refinement for microgravity flow simulations

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1 Introductory comments

This research involves contributions in the areas of: finite element methodology, nonlinear coupled flow and transport processes, adaptive grid technology for this problem class and parallel computing on PC clusters.

During the current year I have been carrying out research primarily on the coupled flow problem class as well as developing the adaptive library `libMesh` [1] with CFDLab colleagues and performing benchmark studies on the CFDLab cluster and other clusters. This work will continue during the coming year and will include detailed studies related to surface tension driven flows and resulting flow structures for various parameter regimes and boundary shapes, further studies of parallel performance and parallel algorithms, initial studies involving adaptive grid simulations and related efficiency and accuracy studies, and studies of nonlinear dynamics of the evolving flow patterns.

A great deal of progress, as well as several research and academic accomplishments, were made throughout the course of 2003. These achievements may be split into academic and research categories.

2 Academic Progress

As an initial step toward my PhD goals I completed a Master of Science in Engineering degree in May 2003. The requirements for the degree included the creation of a detailed report entitled: A Numerical Investigation of Bénard Convection in Small Aspect Ratio Containers [2]. This report helped consolidate my understanding of the concepts and theory surrounding finite element simulations of fluid flow in thin layers, and will act as an excellent

foundation for the PhD research. The results of this work were presented at the seventh annual United States National Congress of Computational Mechanics meeting (USNCCM VII) in the incompressible flow research symposium [3].

The written PhD qualifying exams for the Aerospace Engineering department were passed during the second week of June 2003. These exams are a week-long endeavor consisting of three individual subject tests in the areas of Analytical Mathematics, Fluid Mechanics, and Aerothermodynamics.

The oral PhD qualifying exam was passed in October 2003. Four professors (including the advisor) examine the student. Questions of a fundamental nature are asked, as well as more in-depth questions about the student's research topic. An application for PhD candidacy was submitted following successful completion of the oral exam.

During 2004, additional coursework will be undertaken to complete departmental 'breadth' requirements and gain a stronger understanding of fluid physics in specialized topics related to the dissertation research goals. A course in Nonlinear Dynamics taught in the Physics department will be taken to gain insight into the dynamics of Rayleigh-Bénard-Marangoni (RBM) flow in terms of critical parameters, bifurcations, and chaos. Finally, an in-depth literature review on the stability of RBM flows will be conducted in preparation for work on the PhD dissertation.

3 Research Progress

The flow of an incompressible Newtonian fluid with heat transfer in a thin layer with a free surface can be modeled by the coupled momentum, continuity, and energy equations:

$$\begin{aligned} \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) - \nabla \cdot \boldsymbol{\sigma} - \rho \beta \mathbf{g} (T - T^*) &= 0 \\ \nabla \cdot \mathbf{u} &= 0 \\ \rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - \nabla \cdot (k \nabla T) &= 0 \end{aligned} \quad (1)$$

where $\boldsymbol{\sigma} = -p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ is the Newtonian stress tensor, \mathbf{u} is the fluid velocity field, T is the scalar temperature field, p is the pressure, ρ is the fluid density, μ is the molecular viscosity, c_p is the specific heat, k is the thermal conductivity, t is time, T^* is a reference temperature, and β is the coefficient of thermal expansion.

On the free surface of the layer, the effects of temperature-dependent surface tension (denoted by γ) are imposed in the form of a stress boundary condition. In these simulations, the free surface is constrained to remain planar under the assumption that the capillary number remains small.

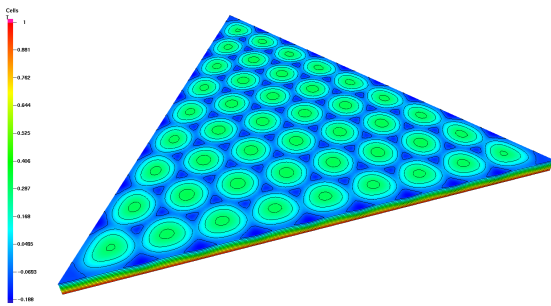
The effect of surface tension is to initiate thermocapillary surface flow from regions of warmer fluid to cooler regions. Polygonal convection cells have been observed experimentally under these conditions by Koschmeider and Prahl [4] and both experimentally and numerically by other authors [5]. One of the goals of the present study is to more fully understand the fundamental fluid physics of these types of flows using computer simulations with high resolution adaptive grids on parallel supercomputers and PC clusters.

Non-dimensionalization of Eq. (1) leads to a corresponding system involving several parameters. The flow regimes which correspond to different ranges of these parameters are of interest. For Rayleigh-Bénard-Marangoni convection, the relevant parameters are the Prandtl number Pr , the Rayleigh number Ra , and the Marangoni number Ma , given by:

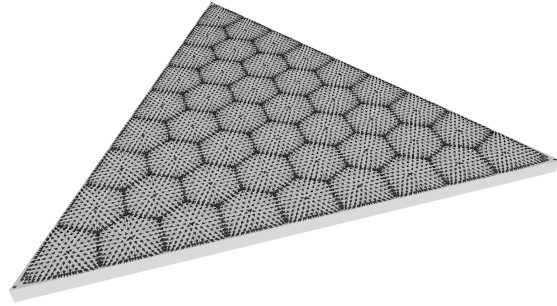
$$Pr = \frac{\nu}{\alpha} \qquad Ra = \frac{\rho^2 c_p \beta |\mathbf{g}| \Delta T d^3}{k \mu} \qquad Ma = \frac{\partial \gamma}{\partial T} \frac{\rho c_p \Delta T d}{k \mu} \quad (2)$$

where $\Delta T = T_h - T_c$ is an imposed temperature difference across the layer of fluid of height d . The aspect ratio Γ of the fluid layer is given by $\Gamma = \sqrt{A}/d$, where A is the area of the free surface.

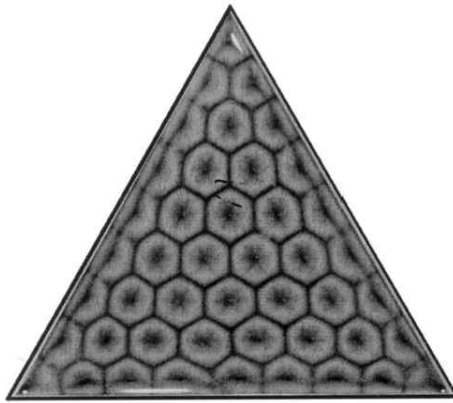
For flows in microgravity environments of interest to NASA researchers, the magnitude of the gravity vector $|\mathbf{g}|$, and therefore the Rayleigh number, can approach zero. Similarly, in terrestrial applications with extremely thin layers, the Rayleigh number approaches zero as d^3 versus d for the Marangoni number. Therefore, these two cases have many important similarities which can be explored. Currently I am examining the effects of container shape on cellular flow structures in terrestrial thin-layer configurations. Representative results are included in Figures 1(a) and 1(b).



(a) Temperature Contours



(b) Velocity Vectors



(c) Experiment

Figure 1: Numerical simulation of Rayleigh-Bénard-Marangoni flow in a triangular domain of aspect ratio $\Gamma = 22$. The Marangoni number $Ma = 105$, Rayleigh number $Ra = 48$, and the Prandtl number $Pr = 913$ in this simulation. The non-dimensionalized temperature contours on the surface of the domain 1(a) and velocity vectors 1(b) agree well with the experimental result obtained by [5] in 1(c). A detailed movie depicting the evolution to steady state of this configuration can be found on the author's web site [6].

4 Future work and conclusion

During 2004 additional Rayleigh-Bénard-Marangoni simulations will be conducted on the new `lonestar` supercluster [7] at the Texas Advanced Computing Center (TACC). Additionally, the computational resources located at Goddard Space Flight Center, especially the Compaq SC45 supercluster known as `halem` [8], should be instrumental in the facilitation of additional simulation work.

I also plan to participate in the GSRP symposium which is held annually at GSFC. This year at the symposium, a ten minute talk on this research effort will be presented. This PhD work is being conducted under University of Texas faculty advisor Graham F. Carey.

References

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