LA-UR-97- - 2572

Approved for public release;
distribution is unlimited

Title: **Low-Speed Flow Hydrodynamics**

Author(s): J. H. Cerutti, X-HM
D. B. Kothe, T-3
S. J. Mosso, X-HM

Submitted to: DOE Office of Scientific and Technical Information (OSTI)

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED *ng*

Los Alamos
NATIONAL LABORATORY

MASTER

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Low-Speed Flow Hydrodynamics

John H. Cerutti*, Douglas B. Kothe and Stewart J. Mosso

RECEIVED

AUG 27 1997

OSTI

Abstract

This is the final report of a three-year, Laboratory-Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). The objective of this project was the inception and development of a new casting simulation tool that is founded in modern, high-order numerical algorithms, accurate physical models, and advanced computational science constructs needed to execute efficiently on parallel architectures. This project has therefore led to the development and application of a new simulation tool (known as Telluride) for the modeling of casting processes used in the manufacture of metal alloy components needed for various Department of Energy (DOE) and Defense Programs (DP) projects. As a result of the efforts undertaken in this project, Telluride can now model key foundry processes in the DOE/DP and in industry. Successes realized over the course of this project have secured funding for further Telluride development by the DOE Accelerated Strategic Computing Initiative (ASCI) Program.

1. Background and Research Objectives

The casting of metals (including alloys) is attractive because it nearly eliminates the energy expended against high flow-stress metals during forging, forming, and machining, which are the alternative fabrication processes for metal components. Casting requires no mechanical work (liquids do not resist distortion), and the energy expended in melting metals is not excessive for melting temperatures under about 1700 degrees Centigrade. The optimum casting is of "near-net-shape," in which all intricate geometric details are cast with enough precision to lessen the need for machining after the part has cooled and been extracted from the mold. Machining waste and the associated safety hazards are therefore minimized. With the thousands of years of experience in casting metal components, it is logical to conclude that the process of casting molten metals and alloys is efficient and well understood. This is surprisingly not the case, as the foundry casting process is still typified by a trial-and-error procedure. Casting today remains an inefficient process, both in terms of cost and energy.

Material microstructural properties of castings are hard to control. A common occurrence is local microstructural variation, which implies compositional and property

---

* Principal Investigator, e-mail: jhc@lanl.gov

variation throughout the entire part. Such defects are extremely difficult to eliminate once they are cast into the part, tending to persist even after final forming. Driven by these increasing demands on quality and control of microstructure, solidification theory and modeling provide the basis for influencing microstructure and improving the quality of cast products.

Casting simulations are cost effective, aid in analysis, and help to advance solidification theory and casting techniques. Only within the last decade, however, has there been extensive research directed at the development of modeling and simulation tools for foundry casting processes. This is in part because of the breadth of complex physical phenomena present in casting processes, ranging from the (possibly turbulent) fluid flow and free surface dynamics governing the mold fill process to the heat transfer and phase change physics important while the part cools. Grain growth and material response (e.g., residual stress) become important as the part cools yet further. In short, casting simulation tools are still in their infancy, as much work in model development and fundamental understanding remains before accurate and predictive three-dimensional (3-D) simulations are commonplace. Such simulations would be invaluable in the foundry.

We have undertaken as part of this project the development of a new casting simulation tool known as Telluride. The principal objective was to evolve Telluride into a comprehensive and robust casting simulation tool that models the relevant processes of fluid flow, heat flow, phase change, solute transport, and interface dynamics, all within the complex 3-D part and mold geometries used in current Los Alamos National Laboratory (LANL) foundries. For Telluride to be able to model LANL casting processes, it must incorporate the latest advances in numerical algorithms, solidification theory, and other physical models.

The modern high-resolution methods developed and used at LANL provided an excellent starting point. An exhaustive list of capabilities was envisioned for Telluride at the start of this project: an unstructured meshing of mold and part geometries, robust and accurate Navier-Stokes solutions based on a collocated finite-volume algorithm, high order schemes for material movement (advection), compact piecewise-linear volume-of-fluid (VOF) scheme for tracking fluid interfaces and solidification fronts, robust and efficient algorithms for solutions of systems of linear equations, physically based models for surface tension and phase change, and diffusive transport for momentum, energy, and alloy species concentration. Most of these capabilities presently reside in Telluride and continued evolution (funded by the DOE ASCI program) will insure that Telluride will indeed reach the full maturity originally envisioned at the start of this project.

Telluride is written in Fortran 90 (F90), where high-level language constructs facilitate modularity, compactness, portability, and extendibility. The source code can execute on any modern computing platform having an F90 compiler, ranging from PCs and single workstations to symmetric multiprocessor (SMP) workstations, workstation clusters, and massively parallel processors (MPP). Efficient parallelization has resulted from explicit message passing through the use of a new parallel gather-scatter library based on the Message Passing Interface (MPI) standard. Parallelization decreases execution time and (more importantly) allows the analyst to perform simulations with higher resolution by applying all available distributed memory to the same problem.

2. Importance to LANL's Science and Technology Base and National R&D Needs

The Laboratory and the DOE/DP complex in general are responsible for the manufacture of many of the metal alloy components found in our current weapons systems. Many of these components are cast, and still more might be cast in the future because casting is typically accompanied by minimal waste generation, reduced exposure and safety hazards, reduced machining requirements and, ultimately, controllable and predictable material microstructure. One potential roadblock to understanding, optimizing, and expanding our current casting processes is the lack of an accurate and comprehensive casting simulation tool. With a simulation tool like Telluride, LANL foundry people and metallurgists can begin to address many casting design issues and procedures before any real metal has to be poured. The current expensive and inefficient foundry practices of "pour-and-pray," trial-and-error castings will be replaced by a series of routine simulations that will aid and guide the casting design process. Given further development of the microstructure models, a simulation tool such as Telluride may also be able to answer (or at least give trends for) detailed microstructure questions such as quantity and distribution of porosity, residual stress, and grain sizes. Given this microstructural information, the metallurgist and materials engineer can develop reliable constitutive models for the behavior and dynamic response of these cast materials as they are subjected to various stresses and strains.

This project directly supports LANL missions for reducing global nuclear danger through stockpile stewardship and support by providing engineers and physicists with an analysis tool designed to help them address important materials issues associated with cast parts in weapons systems. Also supported are the Laboratory core competencies in theory, modeling, and high-performance computing and in nuclear and advanced materials.

The following Laboratory tactical goals have also been supported in this project: science-based stockpile stewardship and management, strategic business development, the plutonium future, integrated environmental science, and modeling, simulation, and high-performance computing. Specifically, through use of the Telluride simulation tool, this project will support the Laboratory goal to establish and certify a process that can be used to manufacture a pit of stockpile quality. This project has also helped to integrate industrial partnership and ASCI research to support the future stockpile's advanced manufacturing requirements.

3. Scientific Approach and Accomplishments

We now briefly itemize our accomplishments during the life of this project. Further detail can be found in the publications generated as a result of this project (cited below) or in the Telluride Home Page at <http://gnarly.lanl.gov/Telluride/Telluride.html>.

- A novel fluid flow algorithm was formulated, implemented, and partially tested (see Publication [12] below). The algorithm is currently an approximate projection method solution of the incompressible Euler equations.
- Our volume tracking algorithm was generalized for unstructured meshes [7]. Two time-integration schemes were implemented: a traditional directionally split scheme and a Runge-Kutta (RK) method. While both are second-order in time (a design requirement), the RK method is much more adaptable to unstructured meshes.
- Efficient algorithms for pure metal and binary alloy solidification were formulated and implemented (Fig. 1). In particular, a new "back-diffusion" model was implemented and tested. This model is attractive because it is void of any unreasonable physical simplifications and it couples nicely to advective transport (i.e., the presence of fluid flow).
- Our volume tracking algorithm was coupled to the fluid flow algorithm, giving Telluride a unique and highly accurate interfacial flow capability. This capability was demonstrated, among others, by difficult free-surface calculations such as a shallow-pool drop splash (Fig. 2) and a box fill (Fig. 3).
- A new "full-remap" volume-tracking algorithm was formulated and tested on two-dimensional unstructured meshes [3,6]. The method utilizes a full remap scheme for time integration, and appears to be the most accurate of all methods we have devised and/or tested to date. Two new methods for computing interface normals from discrete

volume-fraction data were devised and tested in two dimensions. Both methods appear to be the most accurate of all methods we have devised and/or tested to date.

- A model for surface tension (invoked at specified interfaces) was formulated, implemented, and partially tested [5]. This model will be essential for certain mold-filling scenarios and for the direct numerical simulation of dendritic growth.
- An initial set of "mold-filling" simulations was performed. The fluid was assumed isothermal for these simulations (i.e., heat transfer/phase change was ignored), but other conditions such as pouring flow rate were similar to current foundry practices. This capability was demonstrated by a difficult top-fill of a box (Fig. 3) and a fill of a hemispherical chalice (Figs. 4 and 5) that is often cast in the LANL foundry as a test part.
- We performed our first heat transfer/solidification simulation of an actual LANL casting process. Although fluid flow (i.e., the mold fill stage) was ignored for this simulation, we were able to qualitatively predict solidification times for a gravity-pour depleted-uranium cylindrical shell. These simulations were performed in conjunction with another LDRD project.
- A new discrete operator library was formulated and implemented. This module, which makes use of the accurate least-squares methodology introduced by Timothy Barth of NASA/Ames, offers a set of generic operators such as divergence, face-centered gradient, cell-centered gradient, etc., and is currently used throughout Telluride.
- All of the existing algorithms have been efficiently parallelized via coupling to a new parallel gather-scatter library. Subsequent demonstration of parallel implicit heat conduction and phase change on both the IBM SP2 and a DEC SMP Alphaserwer 8400 was extremely successful, with >90% parallel efficiency being realized on unstructured meshes.
- A particle-tracking algorithm was implemented and partially tested on simple velocity fields [8,9]. This algorithm will initially be used for massless tracer particles, but will prove useful for any future particle-based advection of history-dependent variables (e.g., strain).
- We have presented several seminars detailing our project, and we were able to write several papers on various aspects of this project, examples being papers by S.J. Mosso on new 2-D VOF developments and D.B. Kothe on 3-D VOF and surface tension developments. Several papers, however, remain to be written in FY 1997. Topics include our flow and solidification algorithms, parallelization method, and use of F90.

We have also been invited to present our work at several important conferences in 1997.

Publications

1. Rider, W.J. and Kothe, D.B., "Constrained Minimization for Monotonic Reconstruction," LANL Report LA-UR-96-2375, to be presented at the 13th AIAA CFD Conference (1997).
2. Rider, W.J. and Kothe, D.B., "Volume Tracking Reconstructed," LANL Report LA-UR-96-2375, submitted to Journal of Computational Physics (1996).
3. Mosso, S.J., Swartz B.K., Kothe, D.B., and Clancy, S.P., "Recent Enhancements of Volume Tracking Algorithms for Irregular Grids," LANL Report LA-CP-96-227, in Proceedings of the Nuclear Explosive Code Developers Conference (1996).
4. Kothe, D.B., "Computer Simulation of Metal Casting Processes: A New Approach," LANL Report LA-LP-95-197 (1996).
5. Brackbill, J.U. and Kothe, D.B., "Dynamical Modeling of Surface Tension," presented at the Third Microgravity Fluid Physics Conference, NASA Lewis Research Center, Cleveland, OH (1996).
6. Mosso, S.J., Swartz, B.K., Kothe, D.B., and Ferrell, R.C., "A Parallel Volume-Tracking Algorithm for Unstructured Meshes," in Proceedings of the Parallel CFD Conference, Capri, Italy (1996).
7. Kothe, D.B., Rider, W.J., Mosso, S.J., Brock, J.S., and Hochstein, J.I., "Volume Tracking of Interfaces Having Surface Tension in Two and Three Dimensions," Technical Report AIAA 96-0859 (LANL Report LA-UR-96-88), presented at the 34th Aerospace Sciences Meeting and Exhibit, Reno, NV (1996).
8. Rider, W.J. and Kothe, D.B., "A Marker Particle Method for Interface Tracking" (LANL Report LA-UR-95-1740), in Proceedings of the 6th International Symposium on Computational Fluid Dynamics, Lake Tahoe, NV, pp. 976-981 (1995).
9. Kothe, D.B. and Rider, W.J., "Practical Considerations for Interface Tracking Methods" (LANL Report LA-UR-95-1741), in Proceedings of the 6th International Symposium on Computational Fluid Dynamics, Lake Tahoe, NV, pp. 638-643 (1995).
10. Kothe, D.B. and Rider, W.J., "Stretching and Tearing Interface Tracking Methods," Technical Report AIAA 95-1717 (LANL Report LA-UR-95-1145), presented at the 12th AIAA CFD Conference, San Diego, CA (1995).
11. Kothe, D.B. and Rider, W.J., "Comments on Modeling Interfacial Flows with Volume-of-Fluid Methods," LANL Report LA-UR-94-3384 (1995).
12. Rider, W.J., Kothe, D.B., Mosso, S.J., Cerutti, J.H., and Hochstein, J.I., "Accurate Solution Algorithms for Incompressible Multiphase Flows," Technical Report AIAA 95-

0699 (LANL Report LA-UR-94-3611), presented at the 33rd Aerospace Sciences Meeting and Exhibit, Reno, NV (1995).

13. Hochstein, J.I., Fletcher, T.A., and Kothe, D.B., "A Computational Model for Solidifying Flows," Technical Report AIAA 95-0503, presented at the 33rd Aerospace Sciences Meeting and Exhibit, Reno, NV (1995).

Figure 1. Comparison of Telluride simulation results with theory for the propagation of a one-dimensional solidification front (the "Stefan problem") in an aluminum-copper eutectic alloy. The alloy is initially in molten state at its melting point of 821 degrees Kelvin, after which heat is withdrawn from one boundary via an applied temperature of 700 degrees Kelvin. The simulation results are generated with fully implicit solutions of a mixture (solid/liquid) enthalpy conservation equation.

Figure 2. The ability of the Telluride algorithms to model complex topology free surface flows is evident in this simulation of a shallow-pool drop splash. Shown are the drop/pool interface topologies (estimated as one-half volume fraction isosurfaces) at times of 0.0, 0.12, 0.14, 0.18, 0.40, and 0.46 seconds. The 4.0-cm-radius drop, initially centered 3.0 cm above a shallow 2.5-cm-deep pool, is allowed to fall under gravity. The entire system is confined to a 16x16x16 cubic centimeter box. Interfacial surface tension is neglected and all fluids are assumed incompressible and inviscid.

Figure 3. Telluride simulation of the filling of a box from a top corner. Shown are the interface topologies of the filling fluid (estimated as one-half volume fraction isosurfaces) at times of 0.15, 0.25, 0.35, 1.25, 2.0, and 3.0 seconds subsequent to the onset of fill. The 24x24x30 centimeter box is initially occupied with a quiescent background fluid having a density 10 times less than the filling fluid, which is injected with a velocity $\mathbf{v} = (0.0, 0.0, -88.6)$ cm/s through a square hole at the top of the box. Interfacial surface tension is neglected and all fluids are assumed incompressible and inviscid.

Figure 4. Telluride simulation of a pure copper "chalice," which is actually a full-scale mockup of an Au-5% Cu part cast at Los Alamos for the inertial confinement fusion (ICF) program. The chalice casting consists of a hemispherical shell 2.0 inches in diameter. The shell is "gated" at its pole with a cylindrical "hot top" 1 inch in diameter and about 1.5 inches tall. The hot top serves to continuously supply liquid metal to the hemispherical shell during filling/solidification (to avoid shrinkage defects). Shown is a meshing of one quadrant of the mold cavity, assumed to be initially full of quiescent liquid copper at 1270°C. Elements along the two vertical symmetry planes and the top horizontal plane are assumed insulated. For the inner hemispherical surface (adjacent to the graphite mold), a convective heat transfer boundary condition was used with a heat transfer coefficient (h) of 25 W/(m²-K). For the outer surfaces, a coefficient h equal to 15 W/(m²-K) was used, which corresponds to experimental heat transfer coefficient values in stationary air. Shown, from left-to-right, are greyscale images of the solid volume fraction in the chalice at times of 240, 360, and 480 seconds after cooling commences. Regions that are darkest have solidified, regions that are lightest are in the process of solidifying, and regions that are intermediate are still in the molten state. It is obvious from the images that the solidification front is propagating from the bottom and external surfaces of the chalice, as expected.

Figure 5. Telluride filling simulation of the chalice part discussed in Figure 4. For this simulation, the mold cavity is initially filled with a background fluid representing argon gas. At time zero a stream of liquid copper at the centerline having the diameter of the pour hole is introduced from the top via an in-flow boundary condition. The in-flow velocity was about 15.7 inches/sec. Out-flow boundary conditions were applied on the top boundary near the outer edge to allow venting of the background fluid as the mold was filled, since all fluids are assumed incompressible. Shown (left-to-right, top-to-bottom) are the mesh, followed by interface topologies of the liquid copper at times of 0.01, 0.04, 0.08, 0.10, and 0.12 seconds after filling commences.