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Title: **Industrial Applications for the Los Alamos Materials Modeling Platform**

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Industrial Applications for the Los Alamos Materials Modeling Platform

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Abstract

This is the final report of a one-year, Laboratory-Directed Research and
Development (LDRD) project at the Los Alamos National Laboratory (LANL).
Casting and solidification of molten metals and metal alloys is a critical step in
the production of high-quality metal stock and in the fabrication of finished
parts. Control of the casting process can be the determining factor in both the
quality and cost of the final metal product. Major problems with the quality of
cast stock or finished parts can arise because of the difficulty of preventing
variations in the alloy content, the generation of porosity or poor surface finish,
and the loss of microstructure controlled strength and toughness resulting from
the poor understanding and design of the mold filling and solidification
processes. In this project, we sought to develop a new set of applications
focused on adding the ability to accurately model solidification and grain
growth to casting simulations. We implemented these applications within the
Los Alamos Materials Modeling Platform, LAMMP, a graphical-based
materials, and materials modeling environment being created at the
Computational Testbed for Industry.

1. Background and Research Objectives

Casting and solidification of molten metals and metal alloys is a critical step in the
production of high quality metal stock and in the fabrication of finished parts. Control of the
casting process can be the determining factor in both the quality and cost of the final metal
product. New casting methods like slab casting of iron and steel and continuous strip casting
of aluminum and steel can eliminate expensive and energy consumptive steps, e. g., hot
rolling, in the production of a large fraction of the metal stock used by industry. Similarly,

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near-net-shape or final-shape casting of parts can eliminate most of the forging and machining operations that are required in traditional metal manufacturing processes. However, major problems with the quality of cast stock or finished parts can arise because of the difficulty of preventing variations in the alloy content, the generation of porosity or poor surface finish, and the loss of microstructure-controlled strength and toughness resulting from the poor understanding and design of the mold-filling and solidification processes.

Whereas mathematical modeling and even rudimentary computational simulations have been applied to a few of these technical issues by the metals industries, the full range of opportunity for advanced modeling and large-scale simulations to revolutionize the design and development of new casting processes remains largely untapped. For example, in discussions with the staff of the Alcoa Tech Center it has become clear that the major contributor to alloy content and structural property variability in large aluminum ingot castings is the formation of crystal dendrites along the cold walls of the mold, which break off and migrate into and through a mushy solidification layer, sometimes remelting as they pass into the still molten region at the center and bottom of the cooling ingot. This is a highly complex problem in the growth and orientation of the aluminum dendritic crystal structure as well as the multiphase fluid flow, thermal transport, and phase transformation of solid and liquid interpenetrating components. We are well along in developing state-of-the-art, crystal-structure-growth models and multiphase fluid dynamics, and thermal transport codes that can be coupled to form the basis of a general purpose simulation tool for the analysis and enhanced design of bulk casting processes.

With the high cost of creating new materials, any tool that decreases development time offers huge competitive advantages. Modeling has become such a tool, largely due to the great decrease in the cost of computation coupled with large increases in computer power. However, most modeling and simulation is performed with codes designed for specific processes. It becomes a major effort to add capabilities to the codes or to apply them to new processes. We have begun to develop the Los Alamos Materials Modeling Platform (LAMMP), a portfolio of working materials models and materials response and processing codes that is being embedded within a graphics-based environment. LAMMP is being designed so that the user can access modules of differing complexity and link them together in an application tailored to their specific needs. The initial application in LAMMP is a new casting code called TELLURIDE.

In this project, we sought to create new applications for LAMMP focused on developing better and more robust codes for casting, with emphasis on incorporating better materials models within the processing codes. For this project, the specific models describe

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solidification and subsequent microstructural evolution, two factors that play key roles in determining final-state properties of materials.

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

Near-net-shape casting of the metal components of the nuclear package can be an extremely cost effective and environmentally attractive manufacturing processes for stockpile warheads. In addition to weapons manufacturing, the importance to industry of understanding and predicting the development of microstructure during solidification of metallic materials can hardly be underestimated. The tools being developed in this project will have a major impact on our understanding and ability to predict final-state microstructures in cast parts. This project supports Los Alamos core competencies in theory, modeling, and high-performance computing as well as nuclear and advanced materials.

3.   Scientific Approach and Results to Date

There were two parts to this project: (1) creation of new, advanced modeling tools for solidification and (2) implementation of those tools within a coherent platform for casting.

A recent approach to modeling the development of microstructures is to calculate the solidification directly by following the nucleation and subsequent growth of the grains. Previous work [1] focused on isothermal solidification in three-dimensional systems, in which the temperature is constant over the size of sample and where there no heat diffusion. Using a simple nucleation model, they tracked the growth and impingement of individual grains, which were allowed to move through the system. Application of this model was quite successful in predicting reasonable solidification microstructures. However, due to the constraint of constant temperature, it was limited in its applicability to many casting processes.

We have recently implemented a new, more advanced model [2] that incorporates heat flow with detailed microstructure evolution to describe eutectic equiaxed solidification. The basic approach is similar to the earlier three-dimensional model described above. Here, however, we use the microscopic temperatures predicted by the macroscopic heat flow balance in the prediction of nucleation and subsequent grain growth.

The calculations proceed as follows. Given boundary conditions at the edges of the sample (temperature, heat transfer coefficient, etc.) we calculate the temperatures at each node in a mesh using standard macroscopic heat equations and a finite-difference method. We use a linear interpolation to calculate the temperature at all points in the sample cell. Nucleation then occurs with a probability related to the undercooling ($\Delta T = T - T_{eutectic}$) as $n = A_n \Delta T^b$, where

A_n and b are constants and n is the grain density. Nucleation sites are then chosen randomly in the system in a manner consistent with this nucleation law and correspond to new grains with an initial infinitesimally small radius. The radii of any preexisting grains are updated with a simple growth law proportional to the local undercooling. The increase in solid fraction is determined by summing over all area of liquid that has been converted to solid, while keeping track of any impingement of one grain on another. From these microscopic solid fractions, the net macroscopic solid fraction increase at each mesh site is determined and the macroscopic heat equation is used to determine the temperature change at those points. Given the new temperatures at the mesh points, the system is incremented in time and the cycle repeated.

In Figure 1 we show the special grid used in a simulation of the solidification of iron. There are adiabatic boundary conditions on the left and bottom boundaries with a constant heat flux of -60000 W/m^2 on the top and right boundaries. The initial temperature of the melt is 1200 °C and the eutectic temperature is 1154 °C. The transition from gray to white cast iron is not modeled. Shown in Figure 2 are the computed solid fractions and temperatures at the mesh points indicated by the numbers in Figure 1. This is the first model that incorporates a detailed microstructural description of solidification with macro/microscopic heat flow. In the future, we will extend the model to three dimensions, incorporate moving grains, and implement it within a fluid-flow code.

The Laboratory has developed a new fluid-flow code designed specifically for casting. This code, named TELLURIDE, incorporates state-of-the-art meshing with communication libraries that enable use of parallel computing. We have begun to implement new solidification models into TELLURIDE. These are first steps, in preparation for the implementation of the detailed microstructural models described above. We have implemented isothermal phase changes (solidification) for pure materials and for binary alloys. We have tested the accuracy of the algorithm by comparing (for pure materials) the computed results of a one-dimensional Stefan problem (with phase change) with the analytical solution. For binary alloy solidification we used the Scheil rule to calculate solid fraction as a function of temperature and implemented a robust numerical algorithm to update liquid volume fraction (a modified version of Voller's algorithm [3]). We tested the accuracy of the algorithm by comparing the computed results with the semianalytical heat balance integral method of Voller [4].

In Figure 3 we show results from a simulation of the solidification of a Al-4.5%Cu alloy. The mesh was obtained from Alcoa Aluminum and represents one of their test problems. The part was cooled from the bottom. Shown are the volume fractions of liquid, where dark gray is pure solid, light gray is pure liquid, and intermediate shades correspond to regions with both solid and liquid (i.e., mushy zones).

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The principal accomplishment in this part of the project is the first implementation of a state-of-the-art source-based enthalpy method for alloy solidification in a modern (parallel, FORTRAN 90) three-dimensional unstructured-grid simulation tool.

4. References

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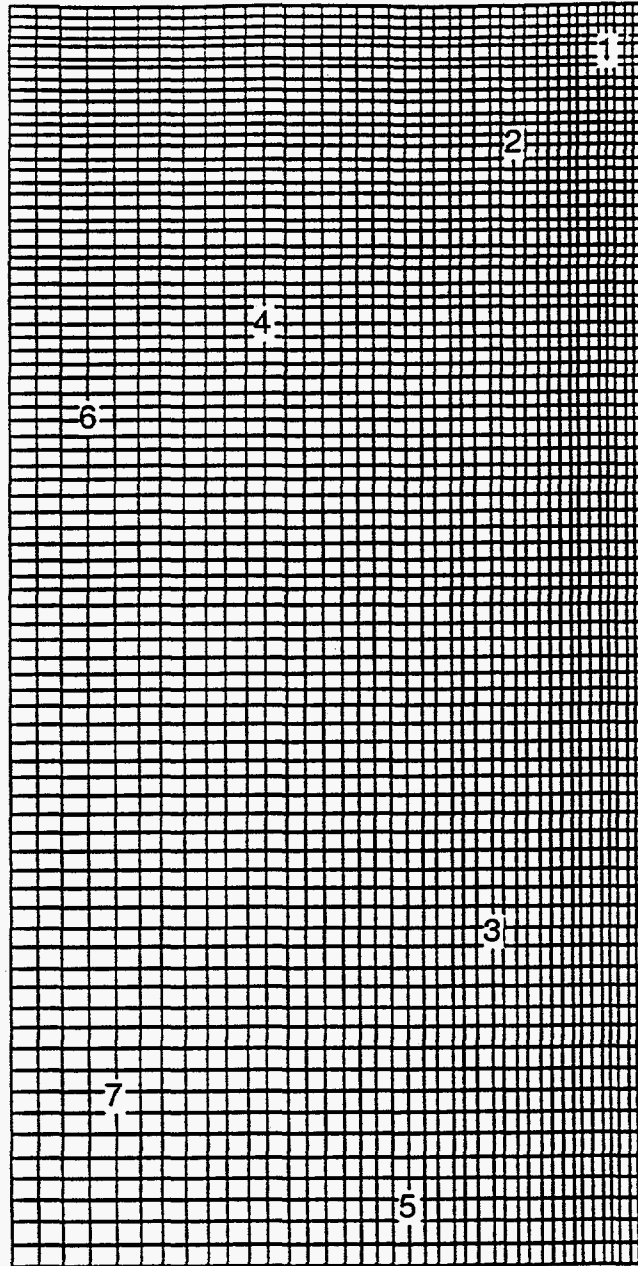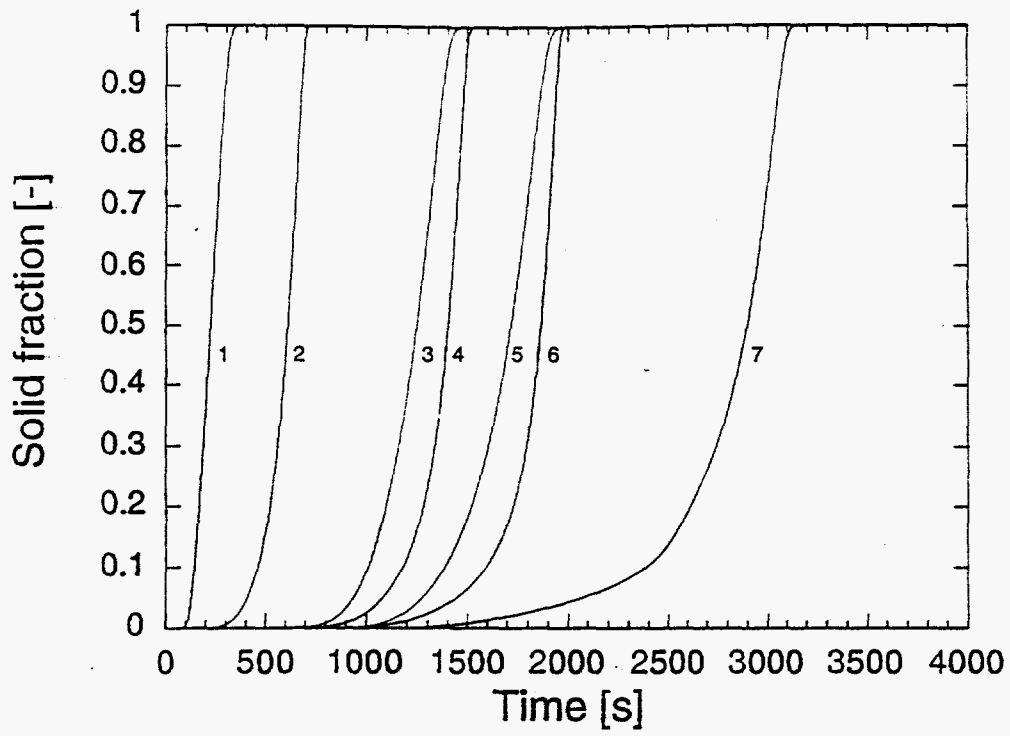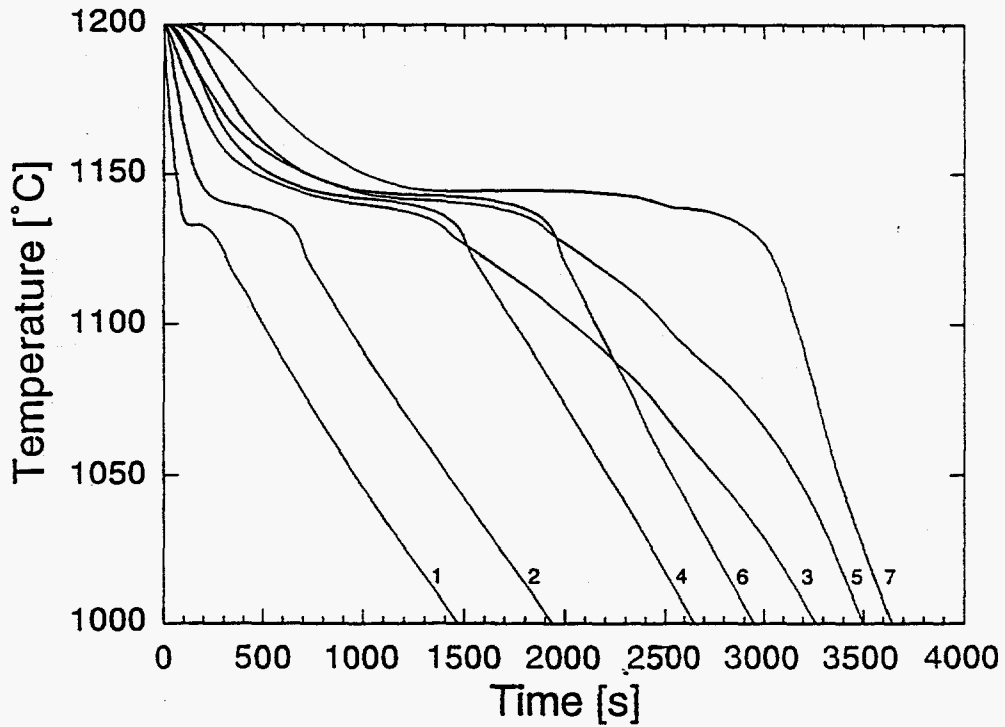
Figure 1. Mesh used in calculation of fully-coupled model of equiaxed eutectic solidification. There are adiabatic boundary conditions on the left and bottom and a heat flux of -6000 W/m^2 on the top and right. The numbers indicate mesh points used in Figure 2.

Figure 2. (a) Solid fraction and (b) temperature versus time at the mesh points indicated in Figure 1.
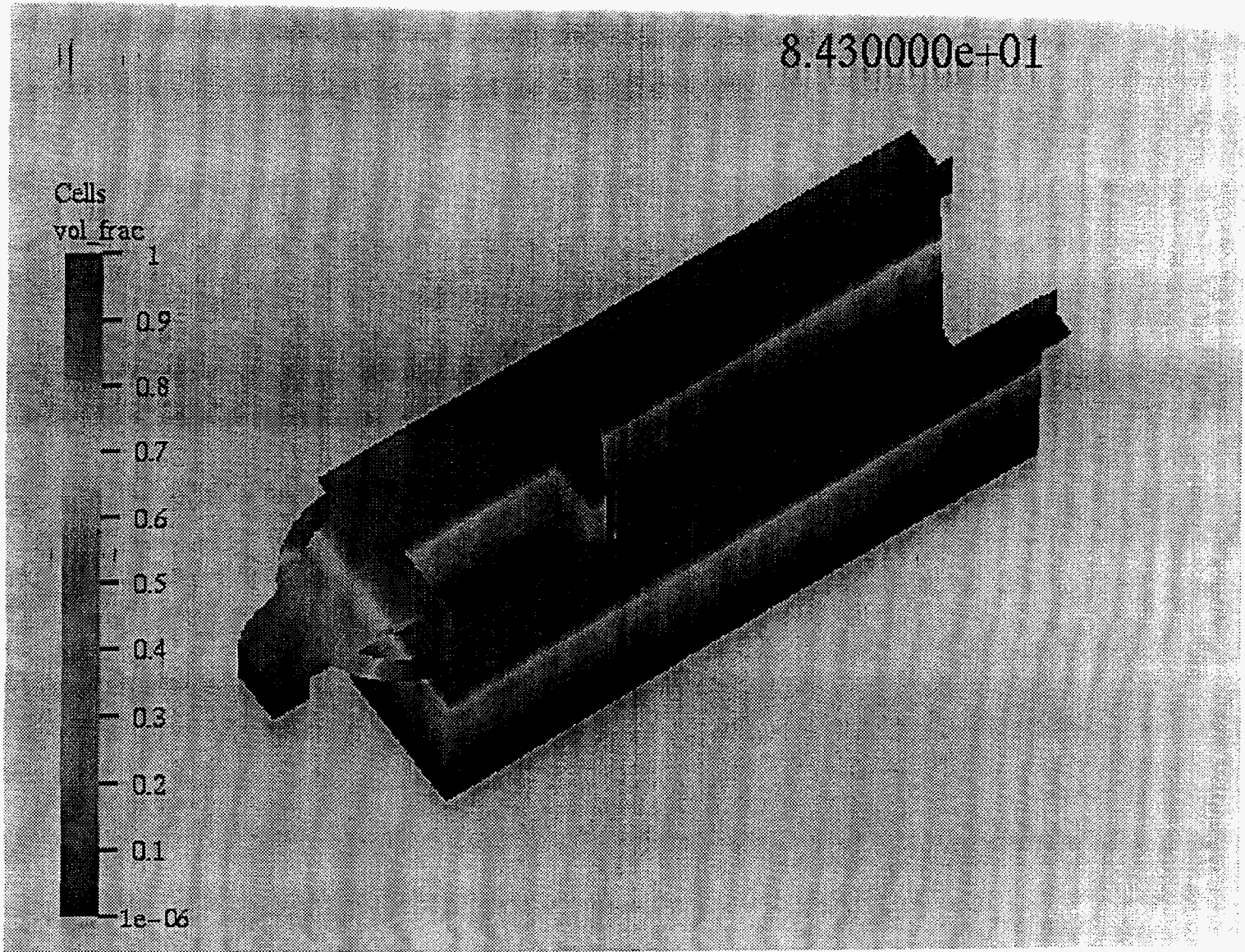
Figure 3. Solidification in Al-4.5%Cu alloy in an Alcoa part. The part is cooled from the bottom, with dark gray areas indicating solid, light gray areas indicating fluid, and intermediate shades a mixture of solid and fluid (i.e., the mushy zone).