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DATELINE: LOS ALAMOS

CASTING CALL FOR MODELS

NEW COMPUTER SIMULATION TOOL WILL HELP FOUNDRIES CAST BETTER METAL-ALLOY PARTS

The Chinese discovered the art of casting copper, bronze and iron thousands of years ago. Today, scientists at Los Alamos use alloys unimaginable by the ancient metal workers. They also have developed a simulation tool to help foundry workers better understand their casting processes. Such simulation tools, especially those capable of running on a supercomputer, were nonexistent a decade ago.

This new computer simulation tool will not only improve the casting process of alloys used in weapons parts, it will be invaluable to private industries that cast complicated metal parts, such as engine blocks.

Los Alamos researcher Doug Kothe stands in front of a plasma furnace with a cast sphere of depleted uranium and its mold. Kothe is helping develop a computer tool that models and simulates the casting process of alloys used in weapons parts. The Telluride simulation tool also will benefit private industries that cast complex metal parts, such as engine blocks.

Researchers at Los Alamos for the first time are modeling and simulating the casting process of metal parts and components produced by Los Alamos foundries. The result is Telluride — a computer tool that models in three dimensions the complex processes involved in casting, including fluid and heat flow, phase changes, solute transports, interface dynamics and material response.

“The potential payoff is enormous,” says researcher Doug Kothe, Telluride development team leader. “The use of computer tools in the area of casting simulation is in its infancy, but the potential cost savings for the Laboratory, as well as industry, are huge.”

For thousands of years metal casting techniques have been

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based on a “pour and pray” method — a foundry term for trial and error. Because many complicated physical processes occur during the casting process, the components often contain flaws that cannot be fixed once cast, and the part must be discarded or remelted. Taking the guesswork out of the casting process will result in less wasted time, money and energy.

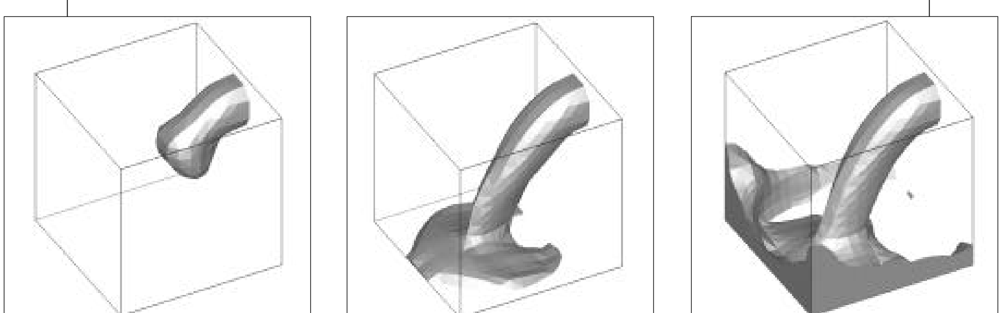
Unlike casting simulation tools currently available to industry, the Los Alamos-developed Telluride code addresses the special needs of the alloys commonly used in Los Alamos foundries: uranium and plutonium. These alloys behave much differently from alloys commonly used in industry, such as aluminum. Los Alamos' casting processes also are unique from those of industry; often involving confined work in gloveboxes.

“We are ahead of currently available commercial casting simulation tools in our ability to simulate smaller and smaller length scales afforded by the Lab’s huge computing platforms,” said Kothe. “We can look at material properties as they happen in the casting process. Our goal is to be able to predict what a cast part will look like at the microstructural level.”

The miscrostructural properties of a cast part are responsible for its strength and resilience, and properly controlling these properties during a pour can minimize defects in the final product.

Telluride metallurgical and software engineers are using the Blue Mountain supercomputer, part of the Department of Energy’s Accelerated Strategic Computing Initiative. ASCI is a collaboration by Los Alamos, Lawrence Livermore and Sandia national laboratories to create modeling and simulation capabilities essential for maintaining the safety, reliability and performance of the U.S. nuclear stockpile in the absence of underground testing.

Six frames from a Telluride simulation of a side pour in a box mold. ↓



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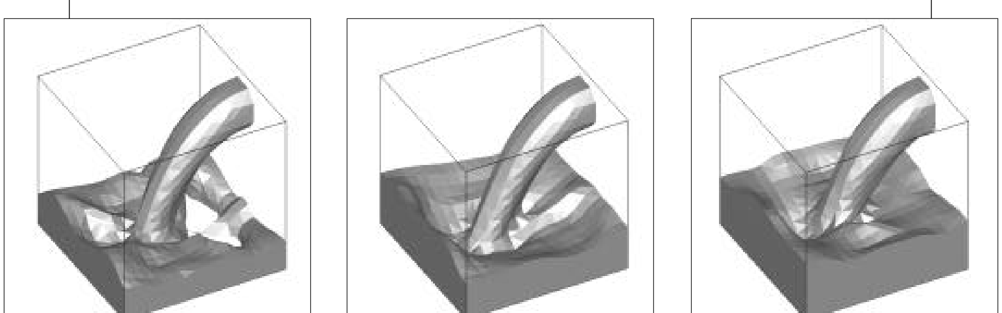
The software is written in Fortran 90 for high-performance computing platforms. Eventually, foundry workers hope to be able to monitor the casting process on a desktop computer and make immediate adjustments to a pour guided by Telluride simulation results. Lab foundries currently are supplying data to Kothe and his colleagues, which they expect to use to validate Telluride on actual cast pieces.

Telluride not only will help minimize "pour and pray" during the actual casting, it will be useful up front in the design process, where it can help design a better mold in a shorter time, thereby reducing mold machining expenses.

Telluride also could have potential in nonmetal castings, such as plastics. This area is yet untested, because Los Alamos does no plastic injection molding but is worth exploring by industry, says Kothe. Telluride's free-surface flow problem-solving skills also may be useful predicting wildfire spread, tracking cloud movement and predicting the impact of "rock-splash" problems, such as tsunamis caused by an asteroid's impacting with Earth.

The Telluride project was initiated with Laboratory-Directed Research and Development funds. Since 1996, the majority of funding has come from the DOE ASCI Program, with additional funding by a collaborative University of California/Los Alamos research program, CULAR.

Current team members include senior project leader Richard LeSar, project leader Doug Kothe, Bryan Lally, Matt Williams and Deniece Korzekwa, Los Alamos' Materials Science and Technology Division; Brian Vanderheyden, Mark Schraad, Mike Steinzig and Frank Harlow, Los Alamos' Theoretical Division; Dana Knoll, Los Alamos' Applied Theoretical and Computational Physics Division; Christoph Beckermann and Jianzheng Guo, University of Iowa; John Turner, Blue Sky Studios, New York, N.Y.; Jeff Durachta, IBM; and Robert Ferrell, Cambridge Power Computing, Ltd.



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An actual uranium pour as seen through the viewport of a furnace. Mica sheet, which serves as insulation, appears in the foreground.

Other contributors have included Jerry Brock, Mike Hall and Jay Mosso, Los Alamos' Applied Theoretical and Computational Physics Division; Janine Fales, Los Alamos' Engineering Sciences and Applications Division; Anand Reddy, Caterpillar Corp.; Roger Rangel, University of California/Irvine; Jean-Pierre Delplanque, Colorado School of Mines; Srinath Viswanathan and Adrian Sabau, Oak Ridge National Laboratory; E. Gerry Puckett, University of California/Davis; Marcus Schmid, University of Munich; Murray Rudman, CSIRO, Australia; and Jong Leng Liow, University of Melbourne, Australia.

Los Alamos researchers are seeking participants from private industry, especially automotive manufacturers, to test an alpha version of Telluride on their industrial casting processes. More information on Telluride is available on the World Wide Web at http://www.lanl.gov/home/Telluride.

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