SCIENTISTS SEE MICROSTRUCTURES IN A NEW WAY

Written by Leah Barbour | Photography by Megan Bean
Even though avid photographers with cutting-edge cameras can zoom in to see the sharp detail of a new Mustang’s engine, they can’t continue zooming in to see the microstructure of its metallic parts. Even the companies that use metal alloys to create engines, frames and the other industrial equipment in modern vehicles don’t have that capability, only possible with microscopy observation of very small samples.

While cameras that take pictures of large objects with microscale resolution are not yet developed, a team of Mississippi State University researchers is attempting to achieve a similar goal in the field of computer simulation: they’re using supercomputers to simulate the solidification of large parts while still capturing the microscopic transformation of metals from liquid to solid, so manufacturers can determine which alloys are most durable and resilient.

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Mississippi State researcher Sergio Felicelli adds to an algorithm that tells supercomputers how to create images of the microscopic transformation of metal alloys from liquid to solid.
The researchers—mechanical engineering endowed professor and MSU Center for Advanced Vehicular Systems associate director Sergio Felicelli, CAVS postdoctoral associate Bohumir Jelinek and mechanical engineering doctoral student Mohsen Eshraghi—have developed an algorithm to simulate the process of metal alloy solidification that exploits the massively parallel capability of current and future supercomputers where the program simulation is distributed among thousands of processors.

“When you have a liquid metal that is starting to solidify, it may have one little point that solidifies first, and then, it begins to branch—primary branches, secondary branches and tertiary branches. These little structures—dendrites—link together,” Felicelli explained.

The dendritic properties of an alloy reveal its characteristics, including shape, size, orientation and composition, and manufacturers who understand microstructures’ composition will be able to create stronger and more reliable parts for engines, frames and products manufactured from alloys, Felicelli continued.

“Understanding and controlling the dendritic growth is critical in order to predict and achieve the desired microstructure and hence, improve the properties of metal parts,” he noted.

Whether the alloys are made by casting, welding or additive manufacturing (where metals are deposited in powder form and melted into layers with lasers), the research team’s work will apply to most kinds of metallic manufacturing for industrial processing.

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Properties of microstructures are so complex that very little work has been done in simulating large-scale alloys’ solidification with microscale resolution, Felicelli said. So many dendrites are created during the solidification process that only supercomputers feature the technology capable of distributing the task among thousands of processors to complete the simulation in a timely manner.

“The algorithm we designed is able to take advantage of the many thousands of processors in a supercomputer. Current solidification models can utilize only a few hundred processors before their performance starts to degrade, but our algorithm is able to efficiently distribute the task among all processors,” Felicelli emphasized.

The algorithm simulates dendritic solidification of microstructures with near perfect scalability, plus it performs the task in a timely, reliable manner, he said.

As supercomputers continue to evolve, Felicelli expects that so too will the simulation of microstructures.

“In a few years, supercomputers will have millions of processors. They keep increasing the capability of computers by adding more processors; hence the key to large-scale simulations is to develop programs and algorithms that are able to use all those processors efficiently. We’ll be able to do computer simulations of large parts and zoom in at any point to observe the resulting microstructure,” he said.

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