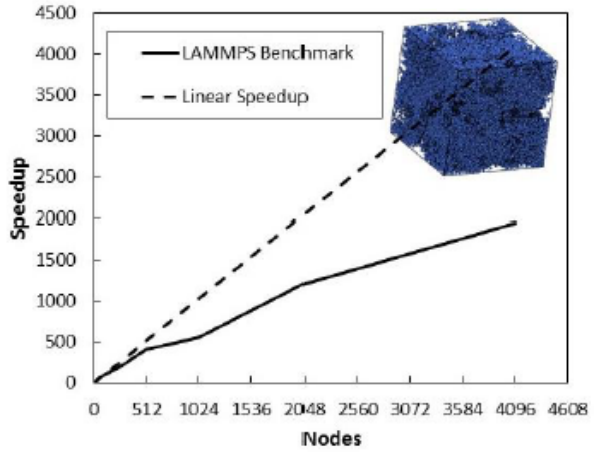
BLUE WATERS
SUSTAINED PETASCALE COMPUTING

Allocation: Exploratory/50 knh
Iwona Jasiuk
University of Illinois at Urbana-Champaign
Physics & Engineering

NOVEL METAL-CARBON MATERIALS

Research Challenge

The team used the Blue Waters supercomputer to model novel metal–carbon materials called covetics, which are metals that are combined with carbon in a new way. Experimental results have shown that covetics have superior mechanical, thermal, and electrical properties compared to base metals. However, the role of the added carbon on materials performance is still not well understood. A goal of this project is to improve our understanding of covetics. This project focused on copper covetics.



The Lennard–Jones benchmark runs on Blue Waters XE6 nodes. The parallel speedup curve is plotted for a fixed-sized test case (strong scaling test) with 200 million atoms.

Methods & Codes

The team conducted DFT calculations on covetics by assuming various copper–carbon configurations. They also employed MD modeling, which has not been used previously on covetics. MD allows them to study larger material volumes due to relatively reduced computational cost compared to DFT and is critical in studying experimentally observed structures. They used LAMMPS classical molecular dynamics code, which has a modular design; the community code model allows users to extend the code at the source level.

Results & Impact

Their initial atomistic and continuum models led to the first predictive multiscale models for covetics, to be published here:

Understanding the influence of carbon addition on the corrosion behavior and mechanical properties of Al alloy "covetics". Varnell, J.A.; DiAscro, A.M.; Chen, X.; Gewirth, A.A.; Bakir, M.; Jasiuk, I.; Nilufar, S.; Journal of Materials Science vol: 54, issue 3, 2019, pp. 2668-2679.

Why Blue Waters

The Blue Waters supercomputer and NCSA researchers were essential for this research project. Blue Waters is necessary because such multiscale modeling requires very high computational resources due to the hierarchical structure of covetics.