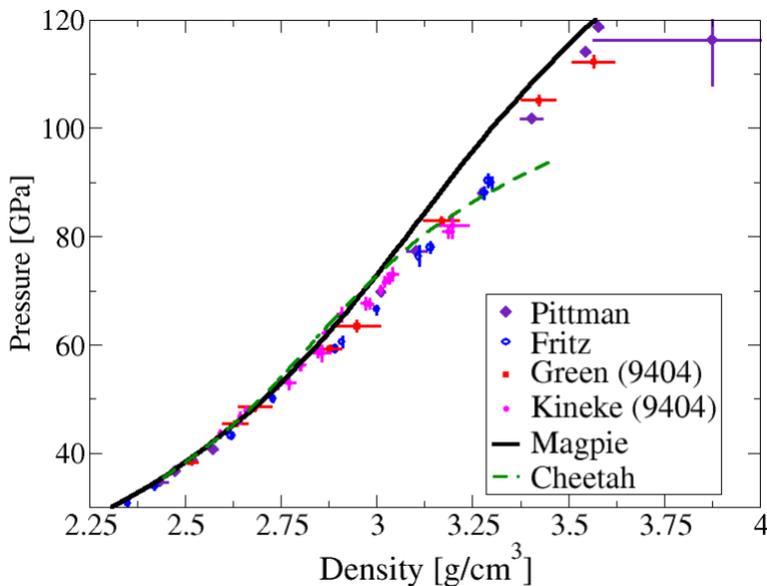


August 2018

Magpie: Reliable High Explosive Equation of State

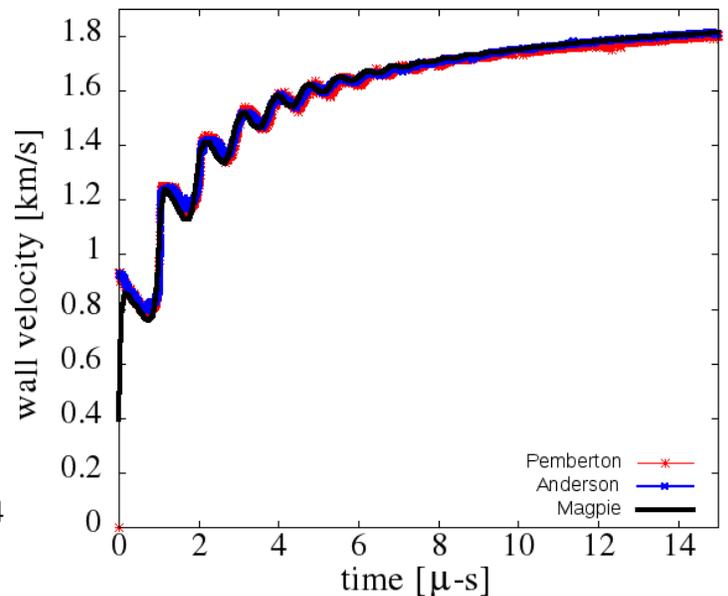
Magpie, LANL's thermochemical code is producing high quality and reliable high-explosive equation of state.

PBX-9501 overdriven Hugoniot



Pressure as a function of density for overdriven experimental gas-gun data compared to thermochemical EOSs. The Magpie result (black) agrees with both recent and historic experiments (points) and with LLNL's Cheetah (green dashed) at lower pressures.

PBX-9501 Cylinder test



FLAG simulation of cylinder test wall velocity as a function of time using the Magpie EOS (black) compared to experimental results from LANL (red, blue).

The Science

Work on Magpie in the Theoretical Division has produced an important fundamental capability to LANL. Magpie now has the ability to predictively generate High Explosive (HE) equations of state (EOS). The code's software design allows for quick and easy implementation of new EOS models. This will allow for advances in EOS modeling of not just molecular fluids, but the EOS of almost any substance. Magpie leverages powerful techniques of equilibrium statistical thermodynamics to build EOSs from microscopic level knowledge of atomic and molecular properties.

The Impact

The new HE-EOSs are now being used by those in GS, DSW, the DDT grand challenge, and V&V efforts at LANL. So, this work directly supports the lab's stockpile stewardship mission. Furthermore, the software infrastructure will now allow cutting edge scientific work, aided by T's ab initio modeling capability to dramatically improve the quality and predictive ability of Magpie and its EOSs.

Summary

LANL now has a world-class thermo-chemical code, capable of competing with other comparable codes. Despite only recently becoming completely functional, it is already beginning to have direct impact on LANL's weapons program. Furthermore, it will enable future development of HE-EOS. Future work will be on state-of-the art EOS modeling of molecular fluids.

Contact

Chris Ticknor, cticknor@lanl.gov and Jeff Leiding, jal@lanl.gov
Physics and Chemistry of Materials (T-1), Los Alamos National Laboratory

Funding

The work at Los Alamos National Laboratory (LANL) was supported by the High Explosives (HE) program in ASC-PEM. Computational resources were provided by ASC.