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Assessment and development of material models based on quantum mechanical simulations

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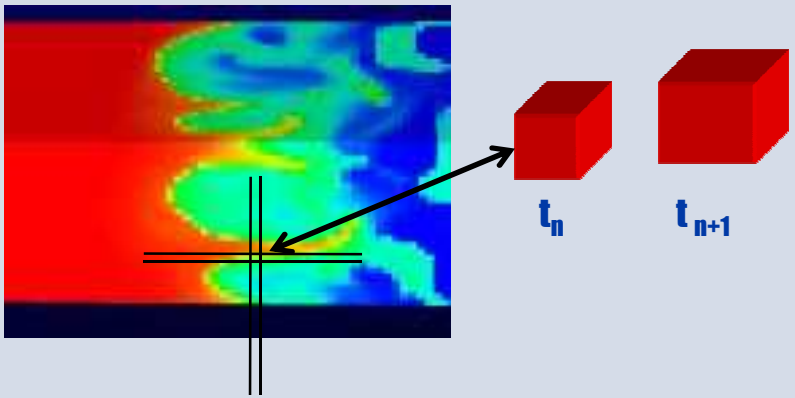
Assessment and development of material models based on quantum mechanical simulations

- High-fidelity material models are essential for establishing a predictive capability for multi-physics rad-hydro simulations
- The quantum mechanics based density functional theory (DFT) and Quantum Monte Carlo (QMC) *provide results without empirical parameters*
- The work supported two level 2 NNSA milestones and one performance incentive in FY11

PI: *Thomas Mattsson*
Code: *qmcpack and VASP*
Run time: *8 cielo days*

Hydrodynamic simulation of shocked foam



In hydrodynamic simulations, the density of the material changes in response to applied pressure and temperature. Knowing the equation of state (EOS), pressure as a function of density and temperature, for each material in the problem, is a requirement for doing accurate simulations.

Assessment and development of material models based on quantum mechanical simulations

- The Density Functional Theory (DFT) code *VASP* is employed to calculate phase-transitions
- Quantum Monte Carlo (QMC), is a higher level theory than DFT
- *qmcpack* scales very well, we ran on up to 73,728 cores and can likely run on all of Cielo
- QMC results are used to correct DFT results and assess the accuracy of quantum exchange-correlation functionals, e.g. LDA

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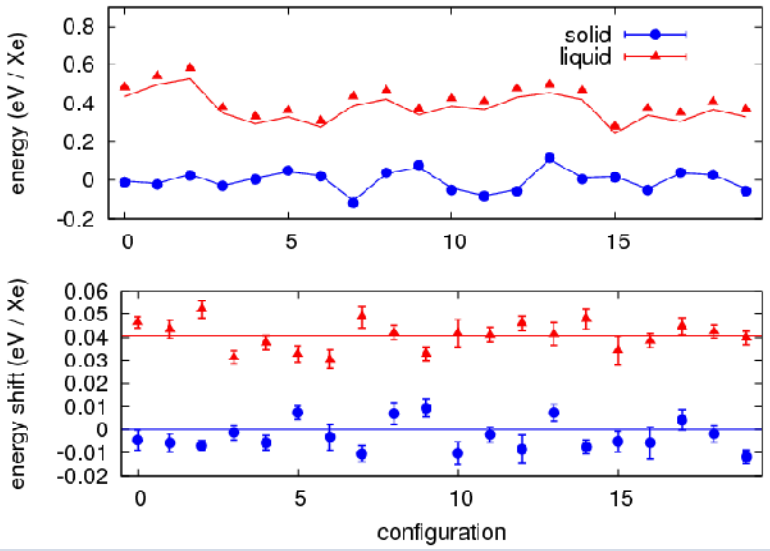
Quantum Monte Carlo Simulations



Internal energy for liquid (red) and solid (blue) xenon at 6000 K and 70 GPa. Comparing results from DFT (lines) with QMC (points with statistical error bars).

From these results, it is possible to apply thermodynamic relations and derive a correction to the high-pressure melting temperature of xenon.

Assessment and development of material models based on quantum mechanical simulations

- The melting behavior at high pressure has been a significant uncertainty in equation of state modeling for a long time
- Different experimental techniques have yielded different results – even qualitatively
- We ran QMC calculations on Cielo, analyzed the melt curve of xenon, and found strong support for a “high” melt line

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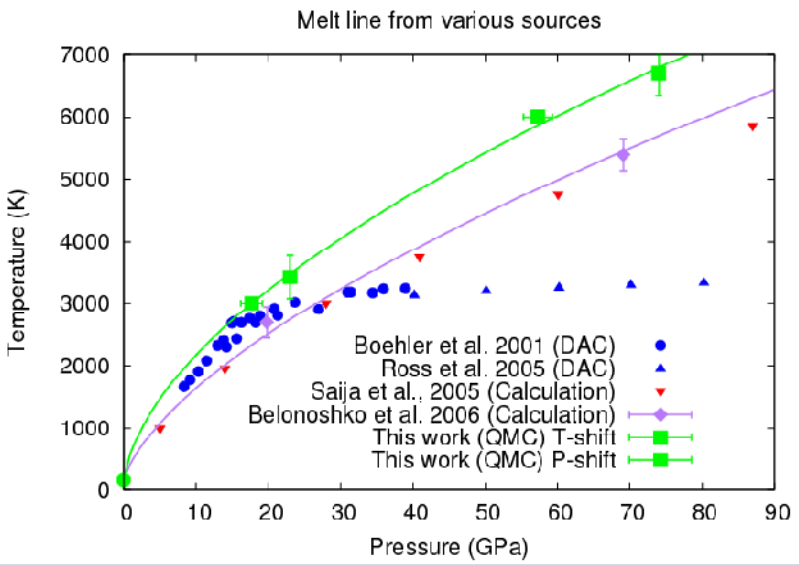
High-pressure melt curve for xenon



There is a long-standing disagreement between experimental results from diamond anvil cells (DAC) and molecular dynamics simulations.

The results from our state-of-the-art QMC calculations strongly suggest that the DAC data should be revisited.

Assessment and development of material models based on quantum mechanical simulations

- The principal shock Hugoniot is one of the most important observables in experiments and ubiquitously used to constrain EOS models
- On Cielo, we performed extensive DFT simulations of shocked argon, making predictions of the shock pressure
- Recent experiments on Sandia's Z machine validated the use of DFT in this regime

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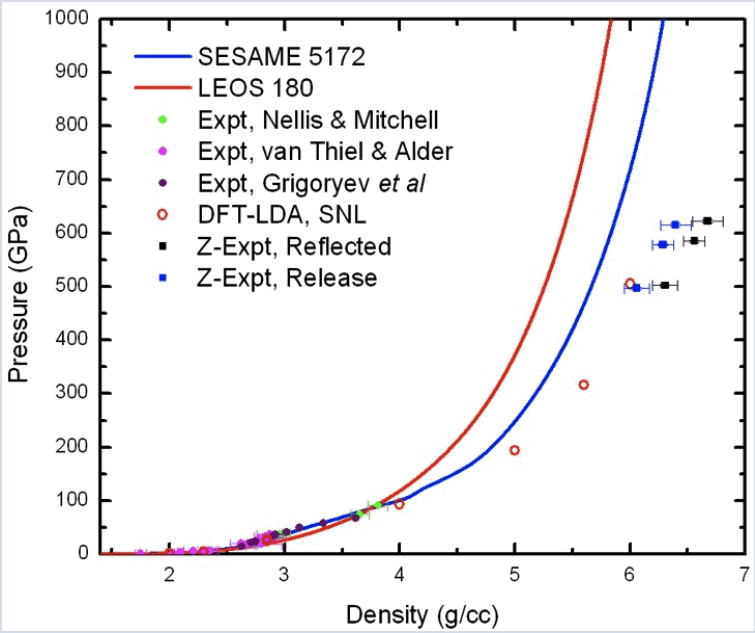
Principal shock Hugoniot for liquid argon



The figure shows the significant differences between the predictions from existing EOS models (LANL blue; LLNL red) and recent Sandia DFT predictions (red circles) and experimental data from Sandia's Z machine (blue circles with error bars).