SAND2015-1325C

A UQ Enabled Aluminum Tabular Multiphase Equation-of-State Model

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Keywords: shock hydrodynamics; equation-of-state; EOS; uncertainty quantification; UQ.

ABSTRACT

To begin to truly understand the boundaries of predictivity in computational simulation, we need to require uncertainty quantification (UQ) in the material models used in the numerical solution of continuum equations. A conceptual framework for the representation and propagation of the uncertainty in the equation-of-state (EOS) for hydrodynamic modeling has been proposed by the authors [1]. The framework includes the use of Bayesian inference to determine the probability density function for the parameters in the EOS models through the use of Markov Chain Monte Carlo (MCMC) methods and the tabular representation of this EOS using principal component analysis (PCA). We have also stressed the importance of an integrated software approach to employing UQ sampling methodologies directly in a continuum modeling code. This work has now been extended to include multiphase models with tens of parameters and multiple phases. We require an advanced adaptive MCMC approach, careful control over acceptable phase boundary shapes in the EOS model, an unstructured EOS tabular format using triangular linear basis functions, smooth mapping of the phase boundaries and interior grids between sample tables to minimize noise in the PCA analysis, and an efficient tabular mesh generation system. Every aspect of the Bayesian modeling coupled with the phase boundary and meshing system must be robust and fast enough to be usable. These requirements are difficult to achieve. We describe the requirements and the solutions found to effectively build a wide range aluminum model using this approach. We also show how the uncorrelated random variables arising from the PCA analysis can be evaluated and understood in terms of probability density shape and independence. For a UQ modeling approach to be effective all material closure properties with significant potential variability should be included in the analysis. The UQ framework described above is thus being extended to include electrical conductivity transport properties and we describe current efforts along these lines.

References

[1] A. C. Robinson, R. D. Berry, J. H. Carpenter, B. Debusschere, R. R. Drake, A. E. Mattsson and W. J. Rider, "Fundamental issues in the representation and propagation of uncertain equation of state information in shock hydrodynamics", *Computers and Fluids*, 83 (2013), 187-193, DOI:10.1016/j.compfluid.2012.10.024.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.