11th. World Congress on Computational Mechanics (WCCM XI)
5th. European Conference on Computational Mechanics (ECCM V)
6th. European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

EFFECTIVE REPRESENTATION AND PROPAGATION OF UNCERTAINTY THROUGH TABULAR MULTIPHASE EQUATION-OF-STATE MODELS

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Key words: *shock hydrodynamics; equation-of-state; EOS; uncertainty quantification; UQ*

A conceptual framework for the representation and propagation of the uncertainty in the equation-of-state (EOS) for hydrodynamic modeling has been proposed and prototyped by the authors [1]. The framework includes the use of Bayesian inference to determine the posterior 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 analyis (PCA). Such a system is important to provide propagation of the uncertainty in data, used to fit the EOS model, up through practical continuum scale computations. Such data may come from experimental sources or first principle model calculations.

We describe the extension of the above work to multiphase EOS 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 mappings of the phase boundaries and interior grids between sample tables to minimize noise in the extended precision PCA analysis and effective use of parallel computing strategies to generate a UQ enabled EOS table. As an example, we describe the development of a multiphase aluminum EOS with an embedded uncertainty representation and then demonstrate its practical use on an interesting shock physics problem.

We have found that an embedded, highly accessible approach at the continuum user level for accessing stochastic sampling methodologies on parallel platforms is a very successful computational paridigm. We will utilize this methodology in our demonstration calculations.

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.

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