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Automated fitting of a semiempirical multiphase equation of state for carbon KIRILL VELIZHANIN, JOSHUA COE, LANL — The equation of state (EOS) of carbon is important in high explosive, geophysical, and inertial confinement fusion applications. Within the semiempirical Sesame framework, the EOS of each phase is represented by a sum of cold, ionic, and thermal electronic Helmholtz free energy contributions. Each phase has 5-10 independent parameters that are adjusted to reproduce single-phase data (e.g., thermal expansion, isothermal compression) as well as experimentally- and computationally-derived phase boundaries. Manual calibration of the full multiphase EOS (i) is arduous, and (ii) complicates (if not prohibits) rigorous uncertainty quantification. We present our progress in development and implementation of automated EOS parameterization based on minimization of a cost function. This function encodes deviation of EOS results from their experimental and computational benchmarks. Optimization is implemented as a combination of global (particle swarm) and local optimization techniques. Accuracy of the resulting multiphase carbon EOS, choice of the cost function, and uncertainty quantification will be discussed.

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