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Numerical Continuation for Atomic and Molecular Fluids

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We wish to obtain accurate structural and thermodynamic properties of both atomic and molecular fluids. Current equations used to describe such quantities have significant shortcomings. In "Optimized theory for simple and molecular fluids" (J. Chem. Phys. 126, 124107, 2007), Marucho and Pettitt propose an improvement upon the existing theory. We present a computational approach to solving this new theory and enable simulations of fluid properties changing as a function of fluid densities. This analysis can be accomplished through a continuation study. We present continuation results using the software package LOCA in Trilinos, a Sandia National Labs solver framework.