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HerEOS: A framework for consistent treatment of the Equation of State in ALE hydrodynamics

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ABSTRACT

We propose a general methodology and practical implementation of arbitrary Equations of State (EOS) evaluation for Lagrangian and ALE hydrodynamic simulations. This approach is based on higher-order interpolations of the Helmholtz free energy (HFE) and derived quantities. We also discuss several pitfalls related to thermodynamic consistency, physical relevance and robustness of the EOS calculations and demonstrate them for realistic values of temperature and density. The developed library HerEOS has been tested and used in various hydrodynamic codes for practical laser plasma simulations, some of which are presented here.

1. Introduction

One of the most challenging issues we face in the simulations of hydrodynamics and laser-plasma interactions is the hydrodynamic closure and proper evaluation of the Equation of State (EOS). To get realistic results that are in good correspondence with experimental data, we have to use physically relevant EOS. Depending on particular range of parameters such as density, temperature and laser intensity, we might need to use various physical models and thus various EOS, sometimes even combine them in one simulation. Among the many existing EOS models and libraries varying in primary purpose, complexity and availability, we generally encounter two types. In the simpler ("inline") case, such as for QEOS [1]/FEOS [2], one can directly obtain values for pressure, internal energy, entropy, and other thermodynamic quantities at any point (say in the temperature–density space), but the calculation may be expensive. EOS of the other type, such as the Los Alamos library SESAME [3], are based on theoretical models combined with experimental data and provided only as discrete values of state variables, with the distribution of data far from ideal. At this point let us remark, that some EOS combine inline and tabulated approaches for different regions.

Our objective here is to develop a tool that allows fast and consistent evaluation of various Equations of State including (but not limited to) ideal polytropic gas, QEOS [1], MPQeos [4], FEOS [2], BADGER [5], and SESAME [3]. This tool, which we will refer to as HerEOS (Hermite-interpolated Equation of State), is intended as a standalone module to be used with various multi-dimensional simulation codes. So far, we have tested our implementation with the 2D Arbitrary Lagrangian–Eulerian code PALE [6] and the multi-dimensional Lagrangian code PETE (Plasma Euler and Transport Equations) [7,8].

Among several reasons to develop such an instrument is the need to reduce the computational cost. In practice, analytical (inline) calculation of a typical EOS, such as QEOS, involves repeated evaluation of complicated formulas and solution of implicit equations leading to the computationally demanding inverse problems. A substantial speed-up can be achieved

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