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CONSISTENT INTERPOLATION OF THE EQUATION OF STATE IN HYDRODYNAMIC SIMULATIONS

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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 physical consistency, relevance and robustness of the EoS calculations and present results of laser plasma simulations using our method in various hydrodynamic codes.

THERMODYNAMIC CONSISTENCY OF THE EQUATION OF STATE

In Lagrangian and ALE simulations for fluid dynamics and plasma physics, involving multi-material flows, laser-matter interactions, heat and radiative transport, etc., we generally encounter two types of EoS. In the simpler (”inline”) case, such as for QEOS/FEOS, one can directly get values for pressure, entropy, etc., at any point (say in the density-temperature space), but the calculations are expensive due to solving inverse nonlinear problems. EoS of the other type, such as the Los Alamos library SESAME, are based on experimental data and provided only as discrete values of state variables, with spacing far from ideal. Both kinds of EoS can be processed by our HerEOS method, using local Hermite interpolation of HFE, as suggested in [1].

In general, we use specific (per mass) Helmholtz free energy $f = \varepsilon - T\,s$, a fundamental thermodynamic quantity, which depends on density ρ and temperature T. Basic thermodynamic (specific) quantities used in hydrodynamics, namely entropy s, internal energy ε and pressure p are defined as

$$s(T,\rho) = -\left(\frac{\partial f}{\partial T}\right)_\rho, \qquad \varepsilon(T,\rho) = f + T\,s = f - T\left(\frac{\partial f}{\partial T}\right)_\rho, \qquad p(T,\rho) = \rho^2\left(\frac{\partial f}{\partial \rho}\right)_T$$

and are complemented by derived quantities such as isochoric heat capacity c_V or adiabatic speed of sound c_s,

$$c_V(T,\rho) = \left(\frac{\partial \varepsilon}{\partial T}\right)_\rho = T\left(\frac{\partial s}{\partial T}\right)_\rho = -\frac{\partial^2 f}{\partial T^2}, \qquad c_s(T,\rho) = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s}.$$

The Helmholtz free energy is a potential, which essentially means that

$$\frac{\partial^2 f}{\partial T\,\partial \rho} = \frac{\partial^2 f}{\partial \rho\,\partial T}, \qquad \text{or, equivalently,} \qquad \frac{\partial p}{\partial T} = -\rho^2\,\frac{\partial s}{\partial \rho}.$$

This property should be respected in real calculations, which is seldom the case. Further physical requirements involve non-negativity of pressure and heat capacity, monotonicity of internal energy and entropy in temperature, monotonicity of pressure in density, equality of internal energy and HFE at zero temperature, etc.

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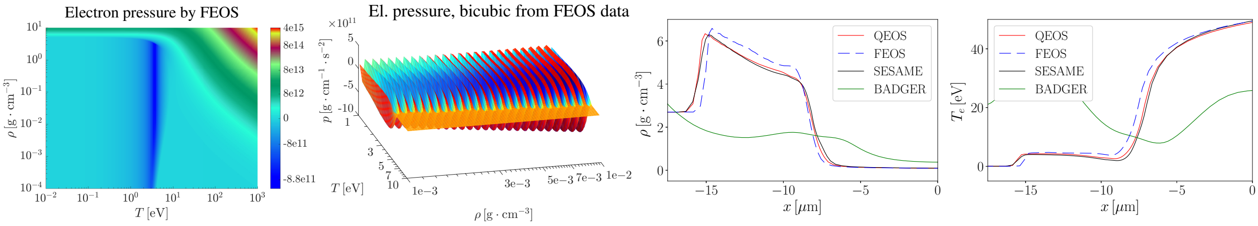

(a) **(b)** **(c)** **(d)**

FIGURE 1: *Data provided by popular EoS libraries may be physically incorrect (a) and/or thermodynamically inconsistent (b). Using various EoS in a simulation yields various density (c) and temperature (d) profiles.*

HERMITE-LIKE INTERPOLATION: IMPLEMENTATION AND DIFFICULTIES IN PRACTICE

The calculations using the HerEOS tool consist of two stages. First, before the actual simulation, the table of HFE and its derivatives (up to the order required for consistency) is constructed for the EoS of choice, using the values of HFE and either utilizing the values of pressure and internal energy (if these are available and consistent), or applying finite differences to HFE. The generated tables can also be stored for further use to avoid repeating this stage in similar future simulations. During the actual hydrodynamic calculation, the values of HFE and its derived quantities (p, s, c_V, ε, etc.) at given temperature and density are obtained easily from the interpolation of the tabulated data.

While sanity checks for trivial EoS (such as perfect gas) yield excellent results and fast convergence even on very sparse interpolation grids, several challenges arise for more physically motivated EoS. Sometimes the EoS libraries we want to utilize contain regions with physically nonsensical values, such as negative pressure (Fig. 1a). Another issue is the thermodynamic inconsistency, that is, provided values of variables such as pressure and heat capacity not corresponding to the derivatives of HFE, which is unfortunately often the case in tabulated as well as inline EoS. In many existing methods, this flaw and consequent issues (such as oscillations of interpolating functions seen in Fig. 1b) are ignored, since the EoS is typically evaluated by thermodynamically inconsistent low-order (bi-linear) direct interpolations of derived variables instead of using HFE. Further inconsistencies appear regarding monotonicity and positivity.

VALIDATION, APPLICATIONS AND FIRST RESULTS

HerEOS has been tested in several multidimensional simulation codes, such as the 2D staggered hydrodynamic ALE code PALE [2] or the Lagrangian code PETE, which includes the nonlocal transport hydrodynamics for laser plasma modeling and is constructed on the high-order curvilinear finite elements library MFEM [3]. Comparison of results obtained with particular EoS types (QEOS/FEOS, BADGER, SESAME) will be given (Fig. 1c-d) and specific numerical issues demonstrated. Finally, results of multidimensional multi-material simulations of laser-matter interaction will be shown, together with their comparison to experimental results obtained at laser facilities PALS (Czech Rep.), LULI (France) and OMEGA (USA).

More information and details about the HerEOS project can be found in [4].

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