Expanding the Tabulated Equation of State Implementations in the FLASH Code for the SESAME Database

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Abstract

We present the enhancement of the tabulated Equation-of-State (TEOS) capabilities of `FLASH` [1], a high-performance computing, finite-volume radiation magnetohydrodynamics (MHD) code developed by the Flash Center for Computational Science. `FLASH` has extended physics capabilities [2] that enable the code to treat a broad range of physical processes in astrophysics, laboratory plasma physics, and high energy density physics (HEDP). Here we extend the tabulated EOS implementation of the `FLASH` code to make use of the SESAME EOS database [1], generated and curated by the Los Alamos National Laboratory. This improvement provides `FLASH` with high-fidelity data for the materials used in laser-driven and pulsed-power driven experiments. We verify the new capability with benchmark HEDP problems and show how they favorably compare against `FLASH`'s previous tabulated EOS implementations.

The SESAME tabulated structure: Strengths and Complexities

Traditionally, an equation of state comprises thermodynamic functions to describe the response of the physical properties a particular material might exhibit under a given set of physical conditions. While an equation might be convenient to program, the physics it can represent can be limited due to the assumptions introduced to formulate it. A tabulated EOS can be more expansive, using a model or combinations thereof to describe thermodynamic properties to varying degrees of physical accuracy [6]. In this respect, a TEOS may offer significant advantages over simpler, analytic EOS.

The SESAME database is a TEOS although rather than solely relying on theoretical models, it is physically motivated [3,4]: experimental data check in different regions the consistency of the thermodynamic interpolations. SESAME involves tabulated equilibrium data [7] in logically-cartesian tables [5], using two state functions (e.g., temperature and density) to populate the phase-space with other macroscopic properties like pressure, internal energy, for 150+ materials.

Therefore SESAME, being publicly available, contains the necessary physics for simulating astrophysical and HEDP systems using `FLASH`. Nevertheless, the database is not fully compatible with the code outright [5]. Data entries may fall into regimes of negative pressures, for which `FLASH` will predict non-physical wave speeds. For this reason, `FLASH` typically initializes a given material at a *higher* temperature to avoid pathologies [7] (see Fig. 1).

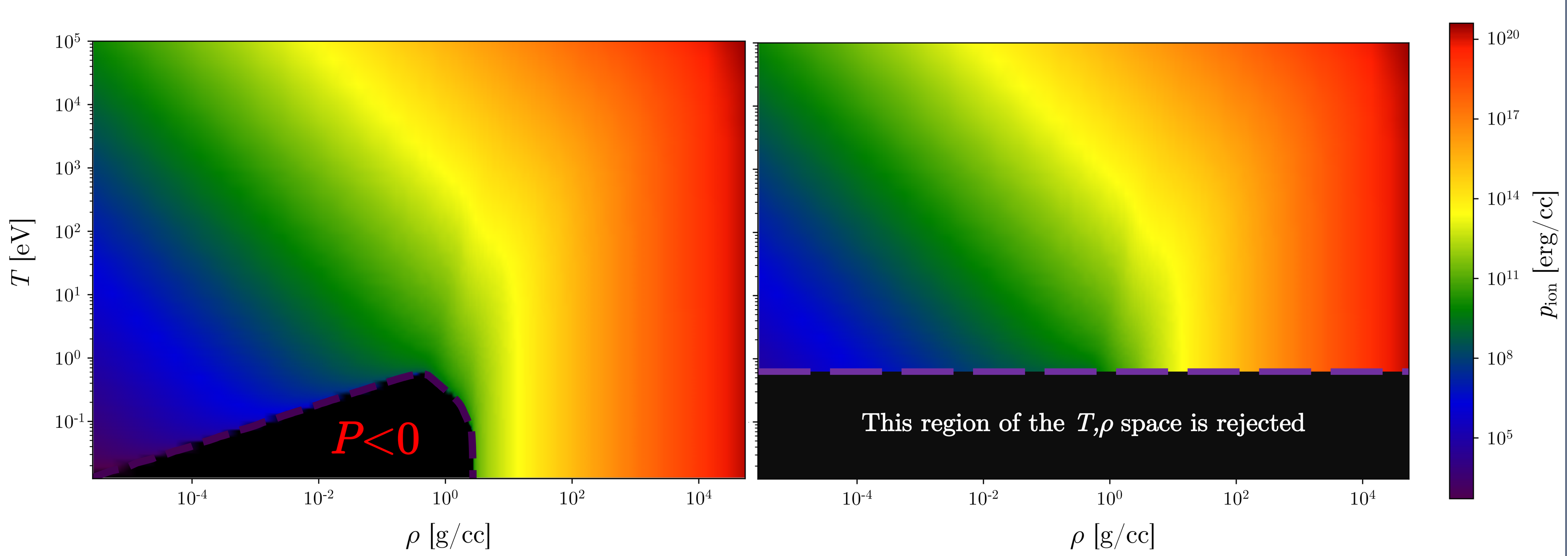

Figure 1. *Example for material 3720 (Aluminum) for the ion pressure. The region containing negative pressures is highlighted on the right, and the current treatment of negative entries is shown on the plot on the right side.*

Interpolation strategy within the `FLASH` framework

The SESAME tables of interest are selected by reading through the material property file to isolate the data associated with specific EOS headers. SESAME provides several TEOS options [4,6]. The framework of the `FLASH` code requires tables 304 and 305, the ion and electron TEOS entries, respectively. The reader truncates the range in the (T, ρ) space, eliminating data of problematic regions, i.e., negative entries. With the working range defined, `FLASH` scans the ranges of the two truncated 304 and 305 matrices to determine their relative orientation.

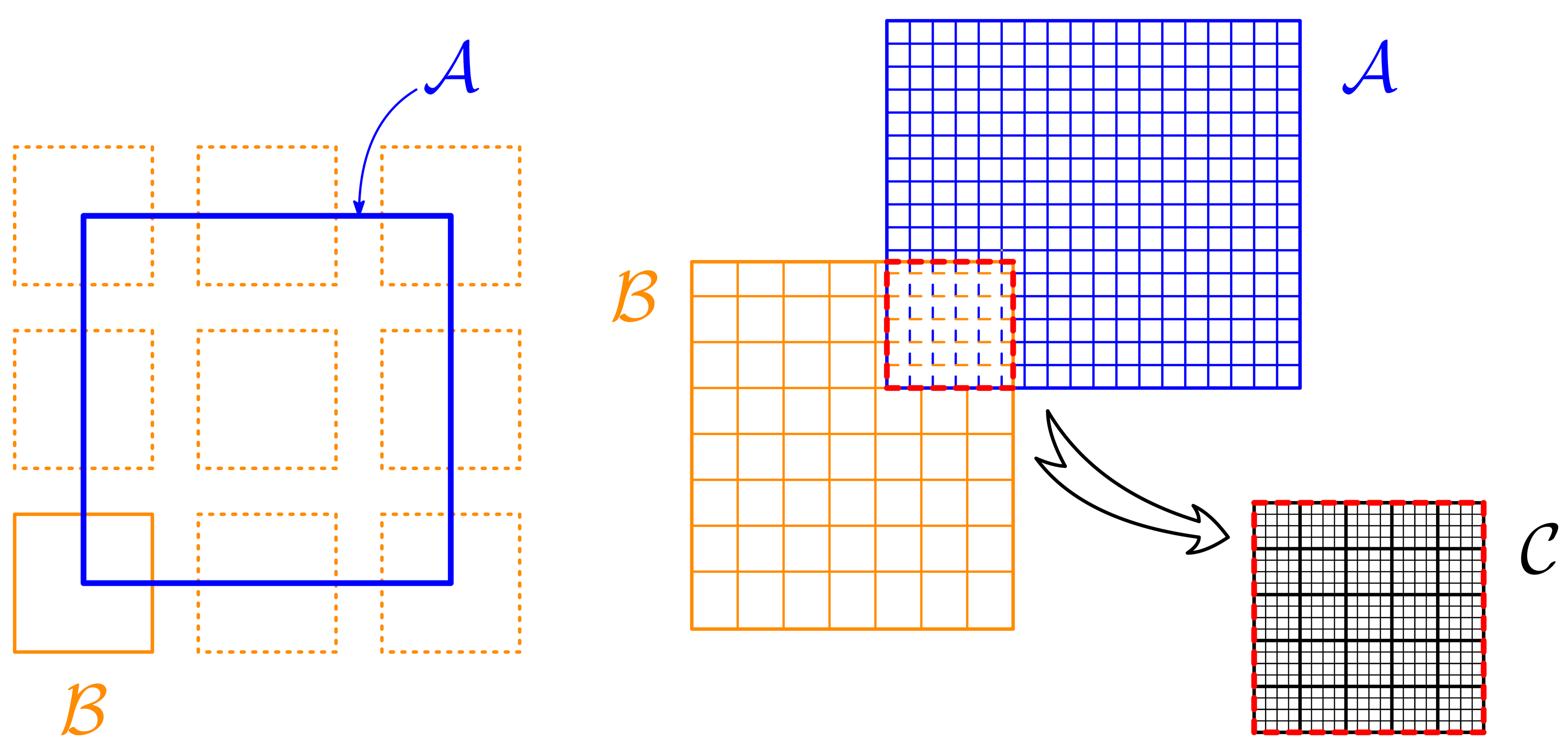

Figure 2. *Illustration of table orientation and the creation of the interpolating grid.*

By determining their relative orientation, `FLASH` can pinpoint the overlapping region in the (T, ρ) space of the concatenated 304 and 305 tables (represented by $\mathcal{A}$, and $\mathcal{B}$, Fig. 2). By implication, this allows the code to establish a common temperature and density envelope for the simulation. The new bounds direct the creation of a new, very fine grid (matrix $\mathcal{C}$, Fig. 2), upon which the physical values of the 304 and 305 EOS tables are interpolated; its high resolution ensures that the derived table accurately captures the profiles of constitutive quantities. Bilinear interpolation is used to populate matrix $\mathcal{C}$ (see Fig. 3 below).

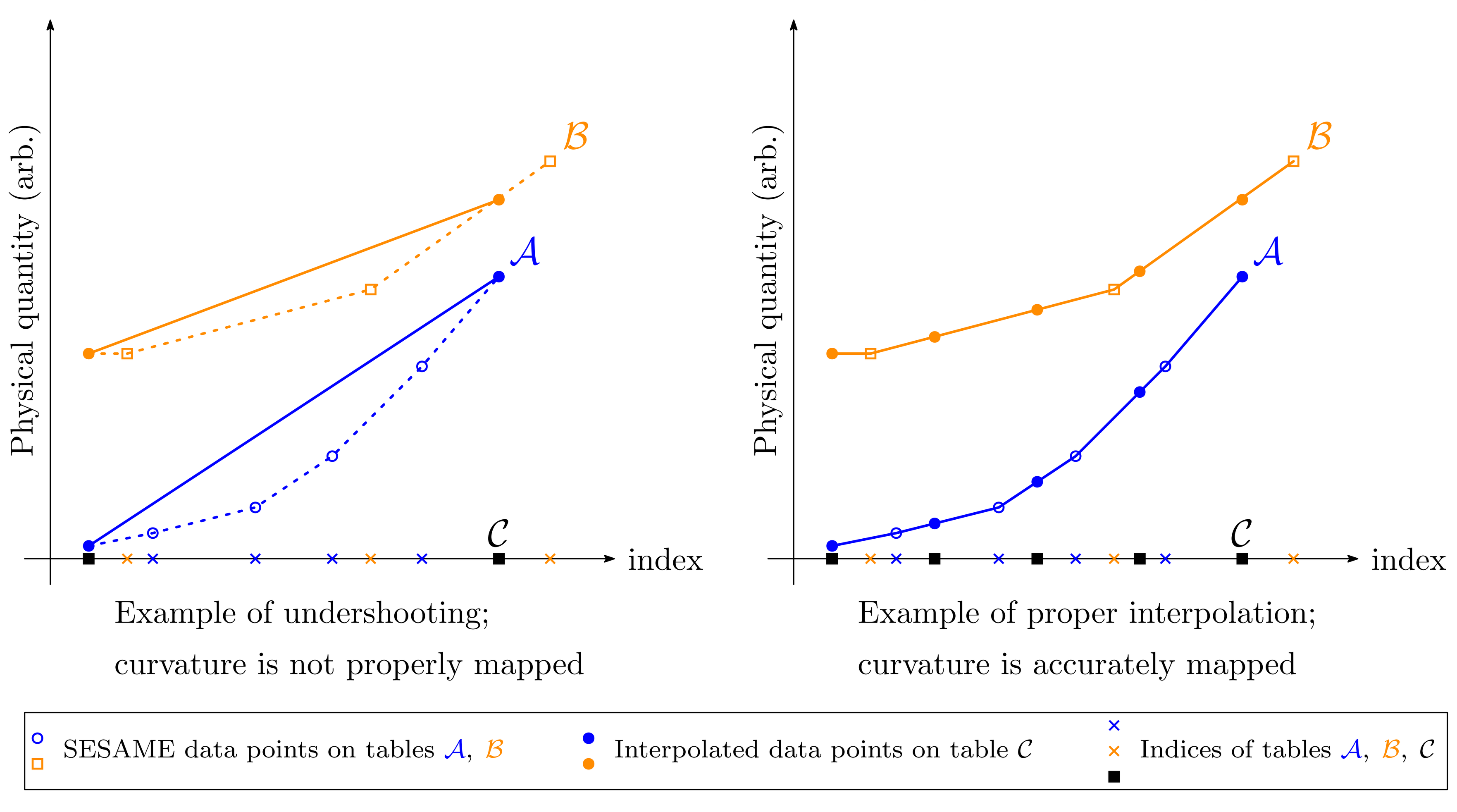

Figure 3. *Schematic illustration of interpolations on a coarse and a fine grid.*

Use of the SESAME database in `FLASH` simulations

The `FLASH` code requires ionization information on top of the thermodynamic quantities provided by SESAME. Thus, interpolating the 304 and 305 matrices using the uniform grid, shown in Fig. 2 as table $\mathcal{C}$, allows the generation of an additional table mapping the ionization of the material across the interpolated (T, ρ) range. Calculation of the average ionization of the material follows the formulary description found in [9]. Using the data from the 304 and 305 TEOS for the material ionization state is a good approximation, as we discuss below.

While this is a first step towards a more complicated EOS description based on first-principles (FPEOS), the strategy has proven to be consistent, and is used in simulations. The implementation described so far offers `FLASH` a native tool to handle SESAME; up until now, FLASH users relied on an external, purpose-built tool, `Opacplot2` [8] to convert SESAME into the CONRAD EOS format that FLASH uses by default. A simulation campaign of 2D cylindrical implosions by Y. Lu utilizes SESAME, as illustrated in Fig. 4.

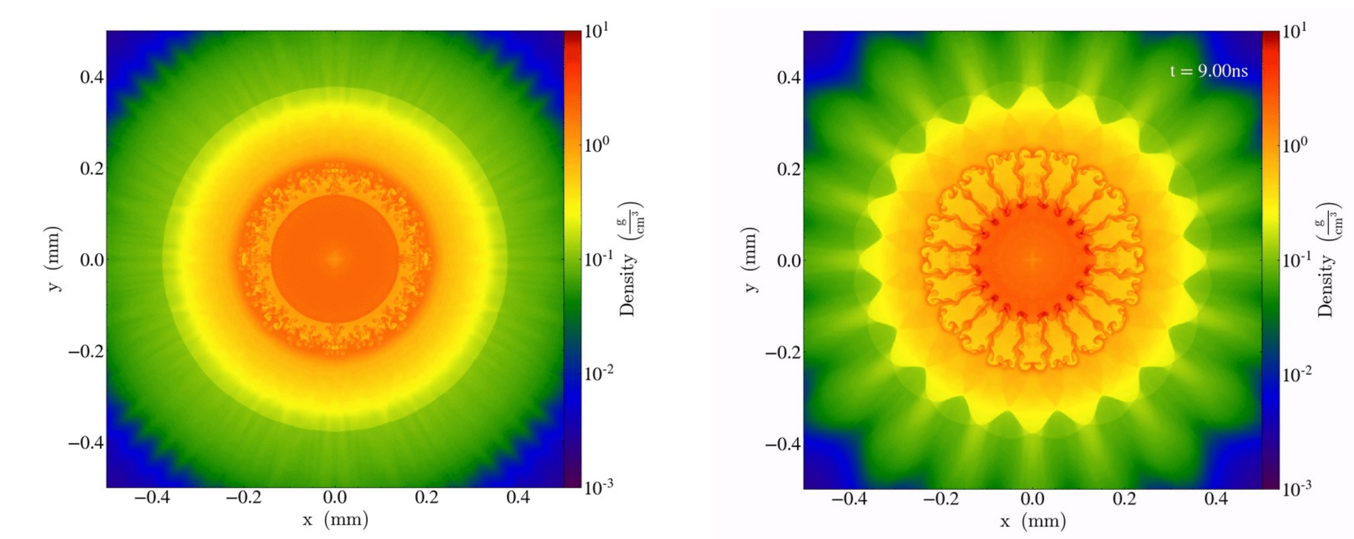

Figure 4. *Density colormaps of 2D cylindrical implosions in `FLASH` using SESAME.*

The development of the native SESAME reader in `FLASH` folds SESAME TEOS into the `FLASH` code development efforts, provides us with opportunities for the further improvements, and enables `FLASH` users to take advantage of the established EOS database developed by LANL.

Future Work

- Expansion of the reader to more material properties tables included in the SESAME database.
- Incorporate the new native reader to the publicly available release of `FLASH`.
- Advance the current work with higher-order interpolation schemes.
- Expand the reader for other TEOS databases sharing SESAME's data format, f.e., an FPEOS package.

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