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ADAPTIVE TABULATION FOR VERIFIED EQUATIONS OF STATE

John H. Carpenter

Sandia National Laboratories, Albuquerque, New Mexico 87185, USA

Abstract. A new adaptive tabulation scheme for multi-phase equations of state (EOS) is described. Adaptation allows verification that a table represents an EOS model to some desired accuracy at a much lower computational cost than standard tables. Computational efficiency is provided through the use of a quad-tree representation. Using both rectangular and triangular interpolation regions results in accurate descriptions of phase boundaries. The new format is demonstrated on a representative multi-phase EOS model.
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INTRODUCTION

Equation of state (EOS) tabulation is a necessity for hydrodynamic codes as all but the most simple EOS models are too computational costly for inline evaluation. As these code are increasingly called upon to provide predictive capabilities, one must account for the uncertainty associated with the EOS model. Tabulation poses a problem as it introduces an additional layer of approximation. By providing a verified EOS table, with a quantified approximation error, one may effectively eliminate this additional layer by ensuring that the tabulation errors are sufficiently less than the errors associated with the EOS model. For example, preliminary investigations have found that the pressure must be verified to better than 5% [1]. Unfortunately, for the standard tabulation schemes such tolerances may require extremely large tables.

Adaptive tabulation provides a means of managing the verification and storage costs by removing unneeded information from a table. At the same time, one may build in other desirable traits, such as thermodynamic consistency and stability along with accurate phase boundaries. An adaptive quad-tree based tabulation has been proposed that conforms to phase boundaries by mapping a single phase region into a rectangle [2]. This is a promising approach except that in general the phase mapping can be computationally costly for state look ups. High-order interpolation [3] and the tuned regression estimator method [4] have been suggested as ways to guarantee thermodynamic consistency. Again, it is not clear that such a guarantee is worth the higher interpolation cost. A redesigned rectangular tabulation scheme that naturally incorporates phase boundary information has also been created [5]. Adaptivity was not included in the design however, so it may suffer similar storage issues as the standard tabulation when performing verification. Building upon these ideas, the goal of the current work is to develop a verifiably accurate tabulation scheme that is computationally efficient in both speed and storage.

SIMPLE MULTI-PHASE EOS

A simple EOS was developed to be representative of typical wide-range, multi-phase EOS models while remaining computationally very simple. To this end, a two-phase system was chosen, with a fluid phase built upon the van der Waals EOS. A solid phase was also included by adding an empirical melting term [6] to van der Waals EOS. The resulting pressure surface is shown in Fig. 1, where the presence of solid, liquid, and gaseous phases are evident along with melt, vaporization, and sublimation regions. This toy

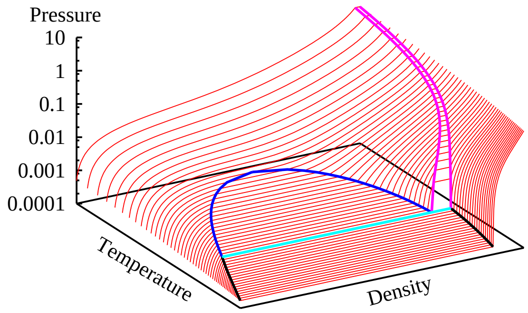

FIGURE 1. Pressure isotherms and phase boundaries of the toy EOS model. The melt curve lies at large density, the vapor dome in the center, and the sublimation region at low temperature. A triple line connects the three regions. Arbitrary pressure values highlight the logarithmic scale.

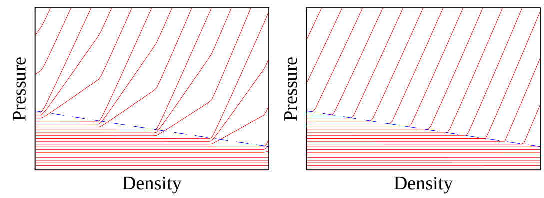

FIGURE 2. Interpolation anomalies in pressure isotherms, shown as red lines. The left plot shows a stair step effect along the liquid side of the vapor dome, shown as a dashed blue line, as obtained from interpolation on a SESAME table. The right plot shows the same isotherms but using the adaptive tabulation scheme.

EOS model is not calibrated to any real system, but exhibits the phase behavior typical of simple metals. The units and values for the model are arbitrary and thus not shown in the plots herein. Furthermore, all plots variables use linear scales with variables increase in magnitude to the right and upwards.

SESAME TABLES

The SESAME tabular format is the de-facto standard for EOS tabulation. It stores EOS data on an arbitrary, rectangular density-temperature grid upon which one tabulates, at a minimum, the pressure and internal energy [7]. To obtain an EOS model one then assigns a particular interpolation scheme to this tabular data. While many types of interpolation may be used, herein we will only use a transfinite Coon's patch with rational interpolation [8].

SESAME tables have a number of deficiencies. Interpolated values may fail to satisfy the first law, $dE = TdS - PdV$, or result in instabilities, $\frac{dP}{d\rho} < 0$ and/or $\frac{dE}{dT} < 0$. The presence of phase transitions often contributes to these issues, due to the discontinuities inherent at first order transitions. These transitions are often poorly represented in the table due to poor choices for the location of grid points, leading to physically stable, but anomalous behavior near transitions. An example of such a deficiency is shown on the left side of Fig. 2 for the toy EOS.

In an attempt to mitigate such issues, a set of best practices has been developed for automatically choosing the grid for a wide range SESAME table to be used with rational interpolation. A similar approach to that of Ref. [5] is used to choose the tabulation grid. First, one chooses a logarithmic pressure spacing for the table, which is applied at the critical density. Typically this will be some division of the pressure range between the triple and critical points. Starting with the critical temperature and pressure, the temperature grid is set to meet the desired pressure spacing at the critical density. Next, whenever an isotherm crosses a phase boundary, the coexistence densities are added to the density grid. The critical density and reference density are also included. Lastly, one augments the density grid with points to ensure that each isotherm contains an interior point in a mixed phase region, and that a certain minimum spacing goal is met for the density grid.

A key motivation to this work is the lack of verification for the interpolated values of SESAME tables. Typically, an EOS modeler will check that certain paths, such as the Hugoniot, are close to the original analytic model, but verification of the complete table is almost never performed. Instead, EOS modelers tend to increase the table density until they feel the table is accurate enough. As a side effect one is often left with very large table sizes.

ADAPTIVE TABULATION

To overcome the issues surrounding SESAME tables, a redesign appears necessary. Adaptive grids provide a promising solution as one may optimize the grid to mitigate the problems described above. A quad-tree is used as it provides a simple method

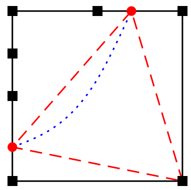

FIGURE 3. Schematic of quad-tree interpolation patch with phase boundary shown as a dotted blue curve. Squares denote the location of quad-tree nodes. With one phase boundary present, the interpolation is split into the four triangles shown by red dashed lines, with additional interpolation points shown as red circles.

of adaptivity with a fast look up speed. The algorithm proceeds as follows. For each rectangle in the quad-tree an error measure is calculated. The rectangle with maximum error is taken as the next one to subdivide. This continues until the maximum error of all rectangles is below the desired tolerance.

The error measure is obtained by sampling the interpolation defined on a rectangle and calculating a three sigma estimate for the maximum relative pressure and internal energy errors. If thermodynamic consistency or instability is detected, the error measure is overridden and the rectangle divided further.

The requirements for the interpolation scheme are that it be computationally efficient, globally continuous, and resistant to instability. For this reason a piecewise bi-linear interpolation scheme was chosen, using a transfinite rectangular Coon's patch with piecewise linear interpolation along the edges [9]. When a single phase boundary crosses the patch, and the error measure using the rectangular interpolation is above the desired criteria, the interpolation scheme is changed. The rectangle is split into four triangles, based upon the location of the phase boundary, see Fig. 3. Then, a similar transfinite Coon's patch is used to interpolate in each triangle. Note, this only affects the interpolation in the rectangle. If the triangular interpolation also fails to meet the error criteria, then the rectangle is subdivided as before.

RESULTS AND DISCUSSION

Two tables were built to represent the toy EOS, an adaptive table with a target verification tolerance of 5%, and a rectangular SESAME table using the outlined best practices. For the latter table, the logarithmic pressure spacing was chosen to give a similar total number of grid points as in the adaptive table. The resultant tabulation grids are shown in Fig. 4. Some statistics for the grids are also shown in Tab. 1. In particular, the rectangular grid contained around 17% more grid points. The nominal number of comparisons needed to find an arbitrary $\rho - T$ point in the grids is also shown. The value for the rectangular table is determined using a standard bisection search, while the adaptive grid value is based upon the average depth of the quad-tree, with the worst case shown in parenthesis.

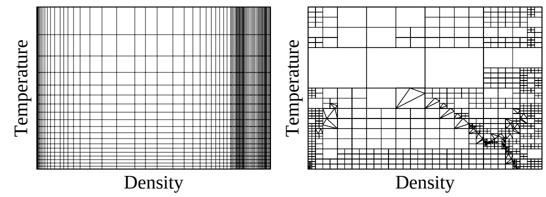

FIGURE 4. Interpolation grids for the EOS. Right and left respectively show a 5% tolerance adaptive grid and a similarly sized rectangular SESAME grid.

TABLE 1. Verification statistics for adaptive tabulation at 5% pressure tolerance compared with a similar sized best-practices, rectangular SESAME table.

Grid type	Adaptive	Rectangular
Total grid points	1404	1640
Look up compares	11 (22)	8
% patches w/ P err $>$ 5%	0.0011	0.328
Maximum P error	0.0544	5.80

To test the verification of the tables, the tabulated $\rho - T$ space was divided into a 1000x1000 log-linear grid. The maximum relative error in pressure was calculated for each of these regions using a random 100 point sample. Some statistics are shown for the grids in Tab. 1 and a visual representation of the error is shown in Fig. 5.

The adaptive grid performs as expected, meeting the error criterion at all but a handful of test locations. When it does fail, the maximum error is still very close to the expected 5%. This is a result of the table generation process, which uses a statistical measure of the error to determine when to stop subdividing. The testing procedure resamples the error on each interpolation patch, and thus it is not unex-

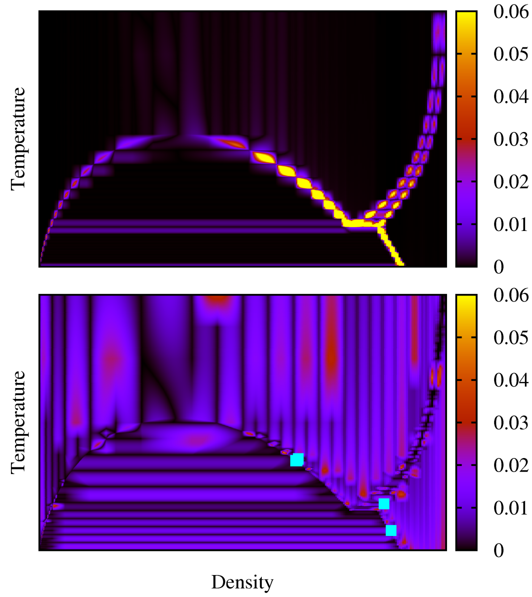

FIGURE 5. Verification results for SESAME (top) and adaptive (bottom) tables. The color gradient shows relative pressure error. Cyan squares in the bottom plot show points where the 5% tolerence was not met.

pected that it may sample the tail of the error distribution differently than when the table was constructed. These results may also be seen in Fig. 5 where the shading shows that the error criteria is met, but typically is close to the 5% limit. The few points where the criteria are not met are shown as squares.

Verification results for the rectangular table are significantly different. As seen in Tab. 1, many more patches fail to meet the error criteria than for the adaptive table. More significantly, when the criteria is not met, the maximum error tends to be much larger, implying the table is much less accurate than the adaptive case in those regions. This is also evident in Fig. 5, where the lightest locations actually lay above the high end of the color map scale. Clearly, the phase boundaries are the troublesome areas. Away from these boundaries the rectangular grid performs very well.

From the perspective of meeting the 5% error criteria, the rectangular grid over performs and wastes storage due to its high density grid. Examining the grids in Fig. 4 shows how the adaptive table overcomes this issue. Grid density is removed, by preventing subdivision where the interpolation is already accurate enough. Additionally, triangular subdivision of the interpolation region allows for the phase boundaries to be accurately captured, unlike in the case of the rectangular grid. Interpolation on a rectangle simply cannot follow general curves with much accuracy. Thus, even upon further refinement of the rectangular grid, the errors at the phase boundaries persist.

Along the phase boundaries the adaptive grid has another significant effect. By more accurately capturing the behavior it restores physicality to the tabulated EOS. This may be seen on the right side of Fig. 2. In contrast to the left side of Fig. 2, the pressure isotherms of the adaptive table do not exhibit the anomalous stair step effect.

ACKNOWLEDGMENTS

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