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Title: EOS Interpolation and Thermodynamic Consistency

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EOS Interpolation and Thermodynamic Consistency

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10/7/11, modified 11/13/15 to add Air example (Fig. 3)

As discussed in LA-UR-08-05451 [1], the current interpolator used by Grizzly, OpenSesame, EOSPAC, and similar routines is the rational function interpolator from Kerley [2]. While the rational function interpolator is well-suited for interpolation on sparse grids with logarithmic spacing and it preserves monotonicity in 1-d, it has some known problems:

1) Thermodynamic quantities are interpolated separately, rather than in a thermodynamically consistent manner, which can lead to thermodynamic inconsistencies.
2) While monotonicity is preserved for the 1-d form, for either of the 2-d interpolation formulas given in [2], regions with monotonic grid values can have non-monotonic interpolants within the 2-d grid.
3) The 2-d interpolation is C^0 (or C^1 for the form given in the appendix), and so thermodynamic quantities calculated from the interpolated values can have unphysical discontinuities.

Form of the 1-d Rational Function Interpolator

Re-analyzing Kerley's 1-d form, one sees it can be re-written as:

f[q] = +f0*(1-q) +f1*q +(df0-f1+f0)*g[q, dg1]

where for Kerley's form g is given by

g_K[q,dg1]=dg1*(1-q)*q/(dg1*(1-q) -q)   for dg1<0
g_K[q,dg1]=dg1*q*(1-q)*(1-2*q)/(dg1*(1-q)+q)   for dg1>0

and where

q=(x-x0)/(x1-x0)
del=(x1-x0)
df0=df/dq|x0=del*df/dx|x0
df1=df/dq|x1=del*df/dx|x1
dg1=(df1-f1+f0)/(df0-f1+f0)

and where f0,f1 are the tabulated values of the function at pts x0,x1, and df/dx|x0,1 are it's estimated derivatives at these points. Note g satisfies the symmetry condition

g[q,dg1] = -dg1*g[1-q,1/dg1]

so the interpolant is direction-independent, and it's behavior is spanned by analyzing -1<dg1<1.

Thermodynamic consistency

From the re-analysis above of Kerley's form one can easily see that for, eg, interpolation of a (Helmholtz free E) as a function of density, instead of using estimated derivates one could use the tabulated values of p (pressure) and da/drho=p/rho^2. The resultant behavior of a and p was shown in Fig 5.a of [1] for Al 3720, reproduced here as Fig. 1.

From Fig 1, one sees clearly that there are problems with the tabulated EOS. There are likely several sources of the problem [3]:

1) numerical issues with TFD,
2) replacing some gridlines with their interpolants, and
3) thermodynamically inconsistent splicing of model regions.

These issues are not specific to this EOS, and these problems are more significant on denser EOS grids. Analyzing the values, it turns out that the minimum and maximum monotonic p interpolants (p=pmin and p=pmax) simply do allow for any monotonic interpolant which satisfies

a1-a0 = int{rho0,rho1} drho p(rho)/rho^2

This indicates there is a need for a quick graphic test to highlight areas where EOS's have problems with thermodynamic consistency for their tabulated values (independent of the interpolation scheme).

Fig. 6 of [1], reproduced here as Fig. 2, showed plots for the Al 3720 EOS highlighting values for the following two tests:

1) a,p consistency:
{ a1-a0 -(rho1-rho0)*(p1/rho1^2+p0/rho0^2)/2 } / {(rho1-rho0)*(p1/rho1^2-p0/rho0^2)/2 }
2) a,s consistency:
{ a1-a0 -(t1-t0)*(-s1-s2)/2 } / {(t1-t0)*(-s1+s0)/2 }

Values of these quantities with magnitudes greater than 1 emphasize regions of the grid where a minimum or maximum in p or s, respectively, would be required to fit both tabulated values, and so no thermodynamically consistent monotonic fit is possible for that line segment. Although a few of the highlighted regions are where p or s are expected thermodynamically to have an extremum, there is significant "stipple" indicating the tabulated points are thermodynamically inconsistent - again, independent of the interpolation scheme.

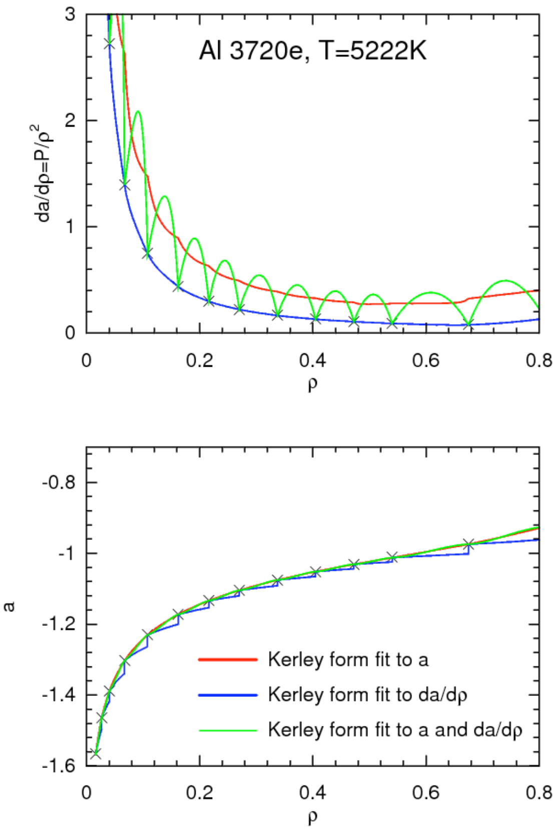


Fig 1. X marks grid points. Comparison of Kerley form fit to a (red) or p (blue) vs Kerley form fit to both (green) for the T=5222K isotherm of Aluminum (sesame 3720). The green curves demonstrates that the tabulated values do not allow for thermodynamically consistent interpolation with this form. Further analysis indicates the inconsistency is independent of the form of the interpolator.

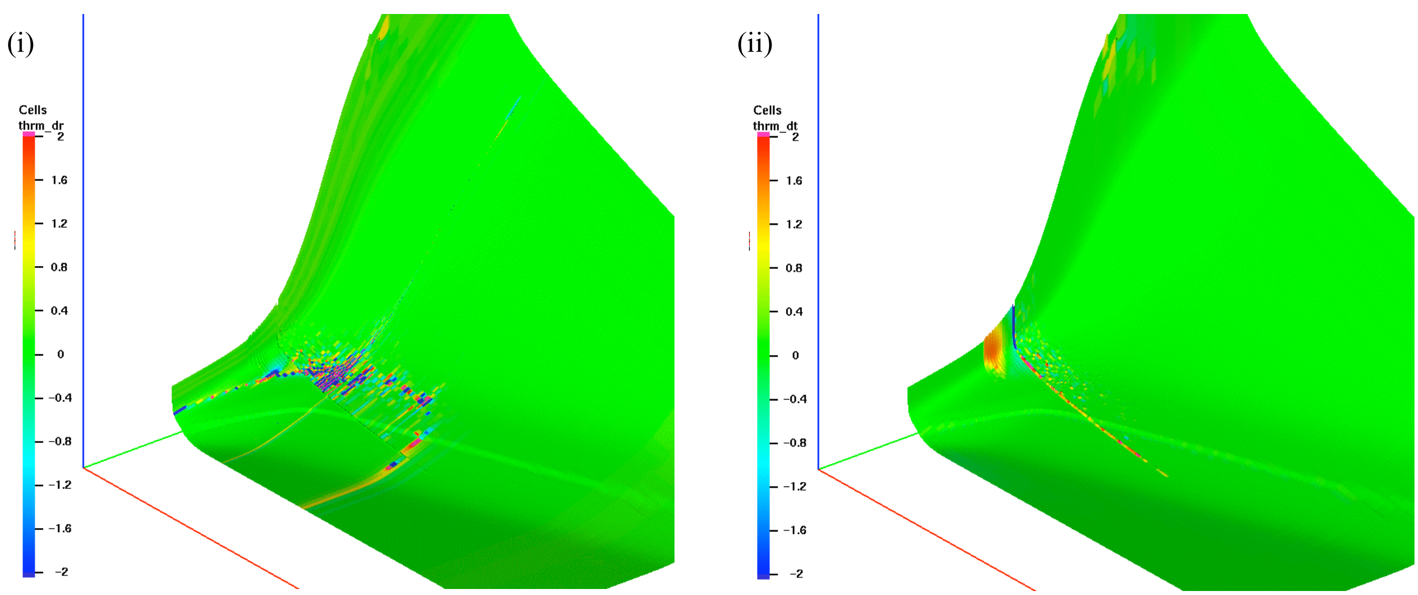
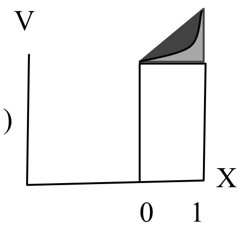


Fig 2. BeO EOS (sesame 7613 with TFD contributions having KGH's corrections) colored to highlight regions (non-green) where the tabulated values of (i) p,a (left) and (ii) p,s (right) require p or s, respectively, to have an extremum. x,y,z values for these plots are r,t,s While not easily visible at this scale, blowing up the p,a relation plot shows a line of inconsistency near rho=rhoref, an artifact of the very dense grid used in that region.

Interpolator-independent thermodynamic consistency tests

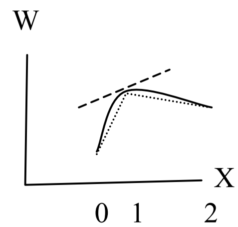
Generalizing the tests discussed in [1] and above, once can define monotonicity consistency test for relations of form V = dW/dX|Y where V,W combinations of tabulated t,rho,p,e,a and X,Y = t,rho or rho,t
Specifically, define
  test_mono = (W1-W0 -(X1-X0)*(V1+V0)/2) / ((X1-X0)*(V1-V0)/2)
where
  W1 = W(t=t1,rho=rho1), etc and Y0=Y1
then if V(X) is monotonic, |test_mono| < 1 if V and W are consistent.



Test compares area needed for integral minus linear fit area (dark grey) to shaded triangle (light+dark grey). V(X) must lie in triangle if monotonic (convex case shown).
Non-monotonic fits can also satisfy |test_mono|<1, so this only tests if a montonic fit is possible for the given tabulated values.

Once can also define smoothness consistency test for relations of same form.
Specifically, define
  dWdX_min = min [(W1-W0)/(X1-X0), (W2-W1)/(X2-X1)]
  dWdX_max = max ["]
  test_smooth = (V1- (dWdX_min +dWdX_max) /2) / ((dWdX_max -dWdX_min)/2)
then |test_smooth |<1 if V at point 1 lies between discrete slopes of W on either side of that point and V and W are consistent.

Specific cases of these tests of interest for SESAME EOS tables and the variables names as currently coded to plot as 3-d gmv files are given below and shown in Fig.s 2 and 3.



satisfying smoothness assumption that dW/dX lies between discrete slopes doesn't rule out non-monotonic regions.

a,p:
Using the relation da/drho|t = p/rho^2 yields
smoothness, monotonicity tests with: W=a, V=p/rho^2 X=rho Y=t.
This is plotted as “thrm_dr” for the BeO EOS 7613 in Figure (2.i), with
thrm_dr={ a1-a0 -(rho1-rho0)*(p1/rho1^2+p0/rho0^2)/2 } / {(rho1-rho0)*(p1/rho1^2-p0/rho0^2)/2 }

a,s (a,e):
Using the relation da/dt = -s = (a-e)/t yields
smoothness, monotonicity tests with: W=a, V=(a-e)/t, X=t Y=rho
This is plotted as “thrm_dt” for the BeO EOS 7613 in Figure (2.ii), with
thrm_dt={ a1-a0 -(t1-t0)*(-s1-s2)/2 } / {(t1-t0)*(-s1+s0)/2 }

Using the relation u = -(T^2) d(a/T)/dT|v yields
smoothness, monotonicity tests with: W=a/T, V=-u/t^2 X=t Y=rho

p,e:
using the relation
  P = T*dP/dT|rho +rho^2*du/drho|T
and defining

```
dpdt_01 = (p1-p0)/(t1-t0)                    dpdt_12 = (p2-p1)/(t2-t1)
dudr_01 = (u1-u0)/(t1-t0)                    dudr_12 = (u2-u1)/(t2-t1)
p_0101 = t1*dpdt_01 +rho^2*dudr_01           p_0112 = t1*dpdt_01 +rho^2*dudr_12
p_1201 = t1*dpdt_12 +rho^2*dudr_01           p_1212 = t1*dpdt_12 +rho^2*dudr_12
p_min=min(p_0101,p_0112,p1201,p1212)         p_max=max(p_0101,p_0112,p1201,p1212)
p_av=(p_max+p_min)/2                         d_p=(p_av-p_min)
thrm_du = (p-p_min)/d_p
```

Then |thrm_du| < 1 if dP/dT|rho and du/drho|T at a given point lie between the discrete slopes on either side of P(t,rho=const) and u(t=const, rho), respectively.
This is plotted as “thrm_du” for the Air EOS 5030 in Figure (3), with thrm_du as defined above.

Additional cases can relatively easily be added to the variables plotted should there be sufficient interest.

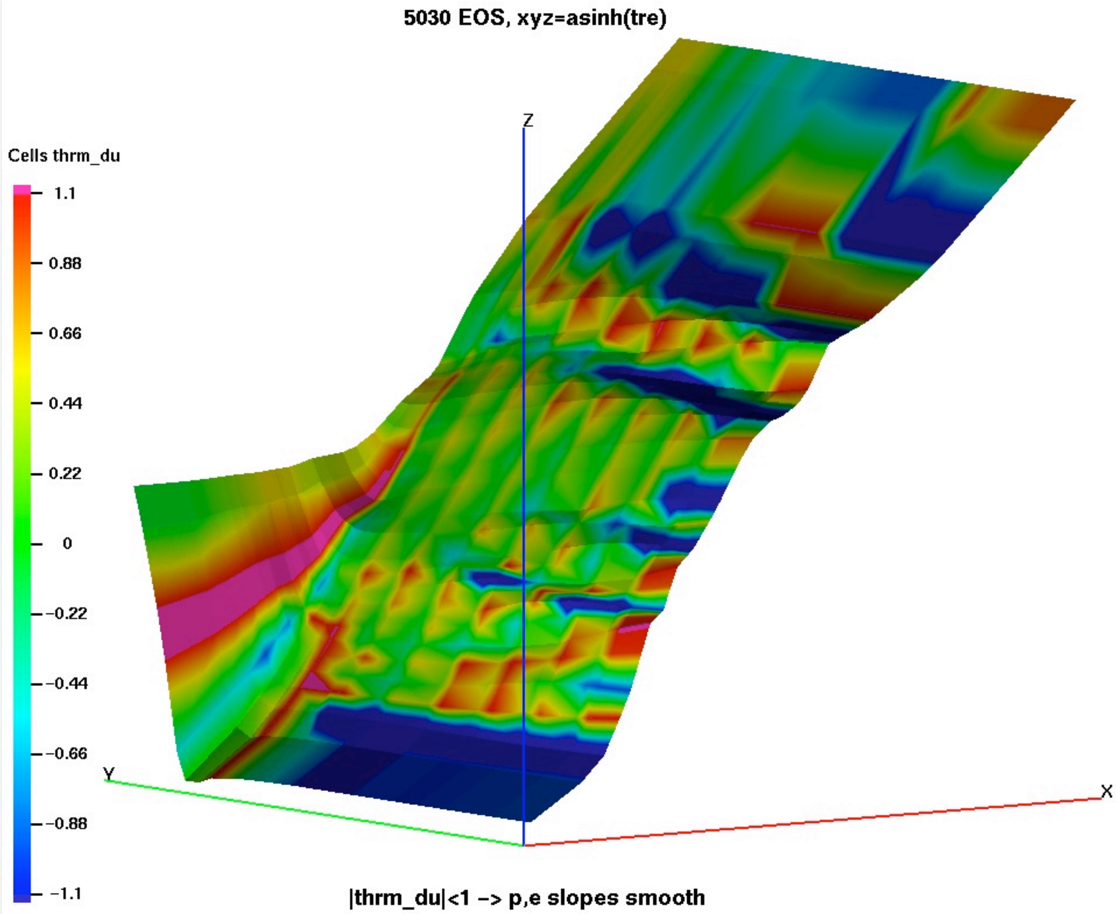


Fig. 3: u(t,rho) for Air EOS (sesame 5030) colored to highlight regions (non-green) where the tabulated values of p,u require at least one of the derivatives dP/dT|rho and du/drho|T to have a local extremum. The plot xyz corresponding to x=x'/max|x'| with x'=asinh(t/RT), y=y'/max|y'| with y'=asinh(r/(1.d-4*rhoref)), and z=z'/max|z'| with z'=asinh(e/.5). Note however this analysis assumes the contribution to the total EOS of the chemical potential can be ignored as at fixed particle number. However, since 5030 is a multiphase EOS, with the percentage of each species varying [4], this "effective single phase" consistency test should be re-examined in the grand canonical ensemble.

References

[1] J.T. Gammel, LA-UR-08-05451
[2] G.I. Kerley, LA-6903-MS
[3] S. Crockett, private communication.
[4] H.C. Grabosky, UCID-16901