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Summary of Modifications to Tabular EOS Material Driver

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Multiscale Dynamic Material Modeling (01435)
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Initial status of tabular EOS drivers

Drivers currently in use:

- Kerley's ("ses" in CTH and "keos sesame" in ALEGRA)
- Kyle's ("snl sesame" in ALEGRA)

Focus on Kerley's driver:

- shared, so improvements available to both codes
- legacy driver, in general used more frequently

Kerley's driver's features:

- Single precision, binary format for tables ($\{P, E\}(\rho, T)$)
- 2-D rational function interpolation (C_0 continuity)
- Hi/low temperature and unphysical tension clips
- (CTH only) out of bounds checks and adjustments
- (ALEGRA only) recomputation of bad sound speeds

Deficiencies of Kerley driver

- Oscillations in the interpolation function
  - Cause energy driver inconsistencies and failures
  - Usually give bad thermodynamic states
- Temperature and energy drivers inconsistent
  - Temperature clipping in energy driver
  - Treatment of off-table energies
- Extrapolation
  - CTH checks give discontinuities in thermodynamic variables
  - “Extreme” extrapolations result in invalid states
- Inconsistent behaviors between codes at extreme states

Improvement goals

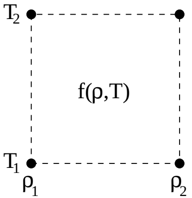
- Provide physically based extrapolation
- Preserve C_0 continuity of the thermodynamic variables
- Reduce bad oscillatory behaviors
- Ensure consistency between T and E drivers
- Create consistency across codes

Greater improvements are needed but do not make sense for legacy tables. As an example take the aluminum 3700 table:

- Kerley table, built in 2003 (“state of the art”)
- Has $\frac{dP}{d\rho} < 0$ and $\frac{dE}{dT} < 0$ (in the grid!)
- Coarse tabulation gives oscillations under interpolation
- Regular grid produces stair-step phase transition curves
- Precision loss causes thermodynamic instabilities

2-D Interpolation 101

Given a rectangular (ρ, T) grid, a patch across four adjacent points is defined by the representation of the function $f(\rho, T)$.



Kerley's driver uses a transfinite Coon's patch:

- $q_x \equiv \frac{x - x_1}{x_2 - x_1}$, $f_{ik} \equiv f(\rho_i, T_k)$, $f_i(x) \equiv f(x, y_i)$
- $f(\rho, T) = f_1(\rho)(1 - q_T) + f_2(\rho) q_T + f_1(T)(1 - q_\rho) + f_2(T) q_\rho - f_{11}(1 - q_\rho)(1 - q_T) - f_{21} q_\rho (1 - q_T) - f_{12}(1 - q_\rho) q_T - f_{22} q_\rho (1 - q_T)$
- $f_i(x)$ are rational interpolants
- patch is C_0 continuous

Rational Interpolation 101

The rational interpolant of $f(x)$ in the interval $[x_0, x_1]$ is:

$$f(x) = \frac{\sum_{k=0}^{3} a_k (x - x_0)^k}{1 + a_4 (x - x_0)}$$

- a_i determined from $f_i \equiv f(x_i)$, $f_i' \equiv \frac{df}{dx}(x_i)$, and $1 + a_4(x - x_0) \neq 0 \quad \forall x \in [x_0, x_1]$
- Interpolant is C_1 continuous (except for $S = f_i'$)

With $S \equiv \frac{f_1 - f_0}{x_1 - x_0}$ one may rewrite f as:

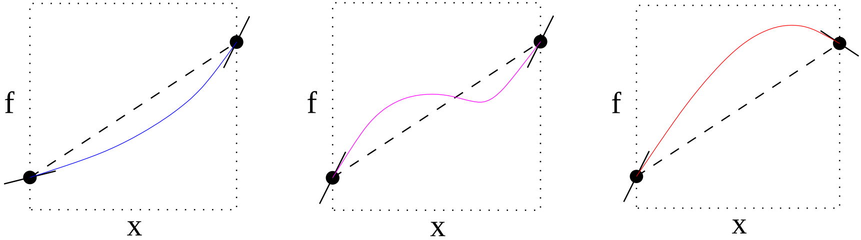
$$f(x) = f_0 + (x - x_0)\left[S - \frac{D_1\mu_1 + D_2\mu_2}{\mu_1 + \mu_2}(x_1 - x)\right]$$

Here D_i are constants and $\mu_i \sim x$.

Oscillation reduction

Three cases:

$0 \lessgtr f'_0 \lessgtr S \lessgtr f'_1$ $\qquad$ $S \lessgtr \{f'_0, f'_1\}$ $\qquad$ $f'_0 \times f'_1 < 0$



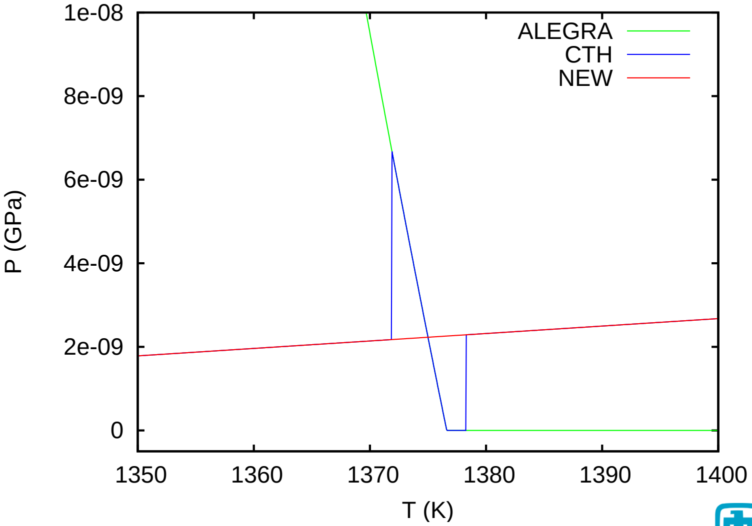
- Only the first case guarantees smoothness
- Third case is tabulation issue for $P(\rho)$ and $E(T)$
- Set $\{D_1, D_2\} = 0$ in second case

$$f(x) = f_0 + (x - x_0)\left[S - \frac{D_1\mu_1 + D_2\mu_2}{\mu_1 + \mu_2}(x_1 - x)\right]$$

- Implemented in SESRTV and SESRVI routines

Oscillation reduction results

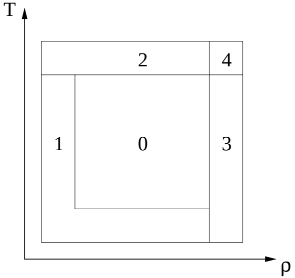
Pressure isochore for Al 3700 ($\rho = 1$ g/cm^3) in transition between unphysical tension region and Maxwell constructions:



Extrapolation strategy

Regions:

1) Generate $T = 0$ and $\rho = 0$ curves
0+1) Interpolate on table
2) Extrapolate to free electron gas
3) Extrapolate to Thomas-Fermi limit
4) Combine extrapolation of 2 and 3



Free electron gas: $F = -F_{EG} T \log(BT\rho^{-2/3})$
Thomas-Fermi limit: $F = F_{TF}\rho^{2/3}$

- Constants F_{EG} and F_{TF} depend only on Z_{avg} and A_{avg}

Low ρ and T extrapolation steps

If absent, add $\rho = 0$ isochore to table, mimicking ideal gas

- $E \sim T$, so let $E(0, T) = E(\rho_1, T)$
- $P \sim \rho T$, so let $P(0, T) = 0$

If absent, add $T = 0$ isotherm to table (here $X \in \{E, P\}$)

- Let $X(\rho, 0) = X(\rho, T_1) - AT_1 \frac{dX}{dT}_1$, with $\frac{dX}{dT}_1 = \frac{X(\rho, T_2) - X(\rho, T_1)}{T_2 - T_1}$
- Choose A s.t. thermodynamic inconsistency canceled near zero pressure, $P(\rho, 0) = 0 = \rho^2 \frac{dE}{d\rho}(\rho, 0)$
- Require $A \in [1/4, 1]$ ($E \sim T^{1/A}$ as $T \to 0$)

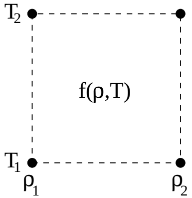
Cold curve tested on legacy tables

- Thermodynamic inconsistency generally within 10% error
  - Assumes A resides in the above interval
  - Many tables behave poorly requiring A to be clipped
  - Typically due to coarse tabulation, ideal gas behavior, or presence of very low temperature isotherm
- $\frac{dE}{dT} > 0$ guaranteed if first two isotherms also satisfy this
- Low T phase transition may cause $\frac{dP}{d\rho} < 0$
- Implemented in SESESI routine

Large value extrapolation

Desire a Coon's patch for extrapolation:

- Need $f(\rho_1, T)$, $f(\rho_2, T)$, $f(\rho, T_1)$, $f(\rho, T_2)$
- As $T_2 \to \infty$ and/or $\rho_2 \to \infty$, $f(\rho, T) \to \infty$
- So, transform ρ and/or T and rescale f



Large T, small ρ:

- $u \equiv 1/T$ and $f_E = \frac{E}{F_{EG}T}$, $f_P = \frac{P}{\frac{2}{3}F_{EG}T}$

Large ρ, small T:

- $v \equiv 1/\rho$ and $f_E = \frac{E}{F_{TF}\rho^{2/3}}$, $f_P = \frac{P}{\frac{2}{3}F_{TF}\rho^{5/3}}$

Large ρ and T:

- $v \equiv 1/\rho$, $u \equiv 1/T$ and $f_E = \frac{E}{F_{TF}\rho^{2/3}F_{EG}T}$, $f_P = \frac{P}{\frac{2}{3}F_{TF}\rho^{5/3}\frac{2}{3}F_{EG}T}$

Large value extrapolation: formulas

Omitted details:

- Use linear forms for speed and to avoid bad behaviors
- Quadratically scale high density to get correct limits
- Utilize table interpolated solution as appropriate
- Transform back to (ρ, T) for simple implementation

Large T, small ρ:

- $E = F_{EG}(T - T_1) + E(\rho, T_1)$
- $P = \frac{2}{3} F_{EG} \rho (T - T_1) + P(\rho, T_1)$

Large ρ, small T:

- $E = F_{TF} \rho^{2/3}(1 - (\frac{\rho_1}{\rho})^2) + (\frac{\rho_1}{\rho})^{4/3} E(\rho_1, T)$
- $P = \frac{2}{3} F_{TF} \rho^{5/3}(1 - (\frac{\rho_1}{\rho})^2) + (\frac{\rho_1}{\rho})^{1/3} P(\rho_1, T)$

Large ρ and T:

- $E = F_{EG}(T - T_1) + F_{TF} \rho^{2/3}(1 - (\frac{\rho_1}{\rho})^2) + (\frac{\rho_1}{\rho})^{4/3} E(\rho_1, T_1)$
- $P = \frac{2}{3} F_{EG} \rho (T - T_1) + \frac{2}{3} F_{TF} \rho^{5/3}(1 - (\frac{\rho_1}{\rho})^2) + (\frac{\rho_1}{\rho})^{1/3} P(\rho_1, T_1)$

Large value extrapolation: final tidbits

Implementation:

- $\rho_1^{1/3}$ precomputed once during initialization (SESESI)
- $\rho^{1/3}$ computed once in SESEOS or SESESV
- Large density extrapolation implemented in SESRT1
- Modification to SESRTV routine
  - Needed table values calculated in original loop
  - Extrapolation applied in additional loop at end
- Modification to SESRVI routine
  - Large T is solved for directly
  - Large ρ utilizes an iterative solve similar to the original

Features:

- Use of table interpolated values gives overall C_0 continuity
- Limit of large ρ and T not well defined
- Clips may still activate at extreme values

Other changes to reverse interpolation

Built in low temperature clip:

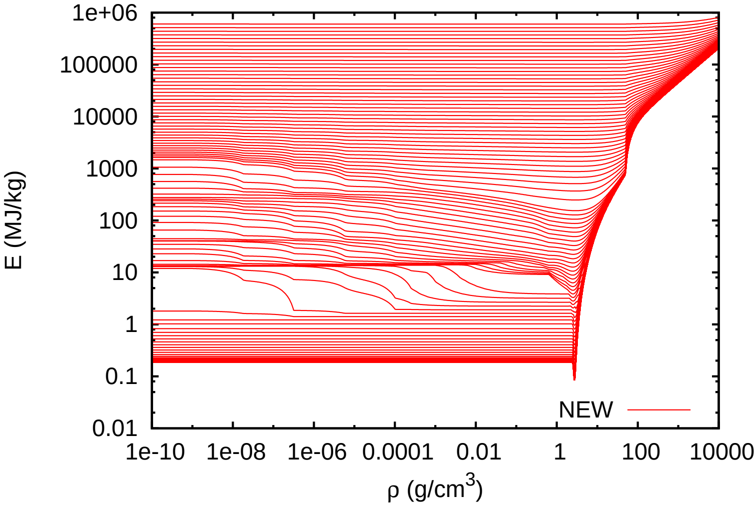
- Gives a consistent state (except for E and $\frac{dE}{d\rho}$)
- Two values $T_<$ and $T_>$ apply when $\rho \lessgtr \rho_{min}$
  - Default $T_>$ is 0.01 K, max is table's T_{max}
  - Default $T_<$ is T of first isotherm with $P > 0$ at smallest $\rho > 0$
  - Prevents return of states in unphysical tension region

Iteration changes:

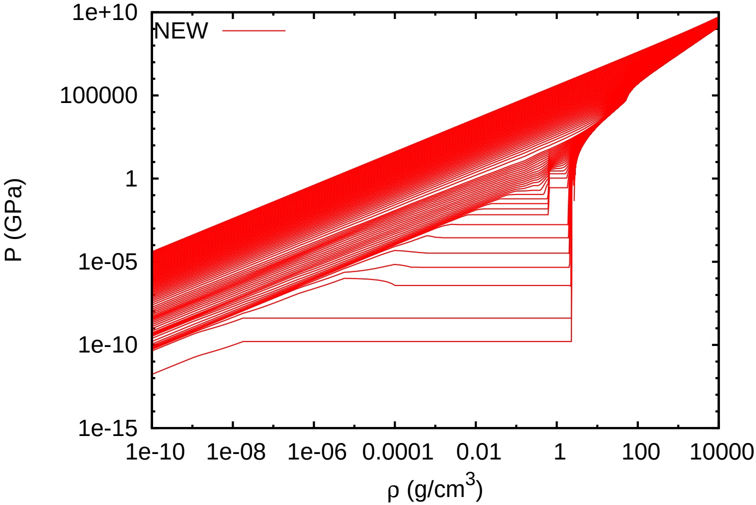
- Bug fix: ΔT should not be added in on loop exit
- Turned off linear fallback for oscillating energy
- Removed Newton method fallback for $\frac{dE}{dT} < 0$
- Added bisection for temperature clipping
- Added temperature convergence test (10^{-3} threshold)

Changes tuned to optimize convergence and give the best consistency possible with SESRTV

Extrapolation results – Al 3700 energy



Extrapolation results – Al 3700 pressure



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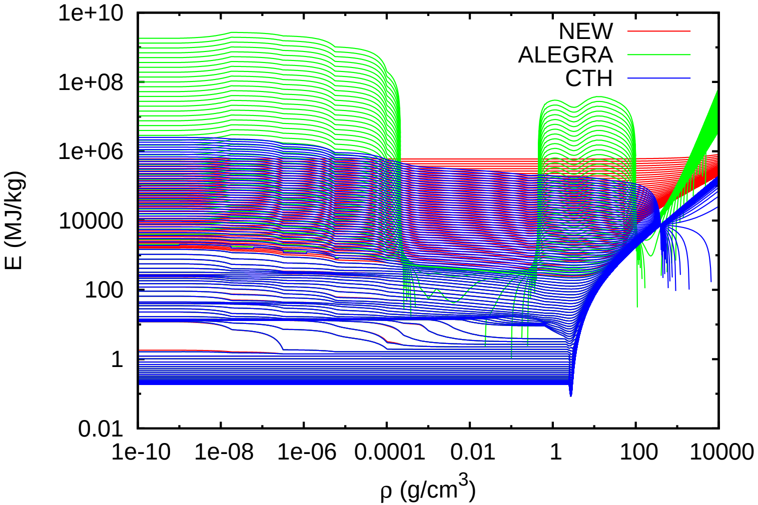
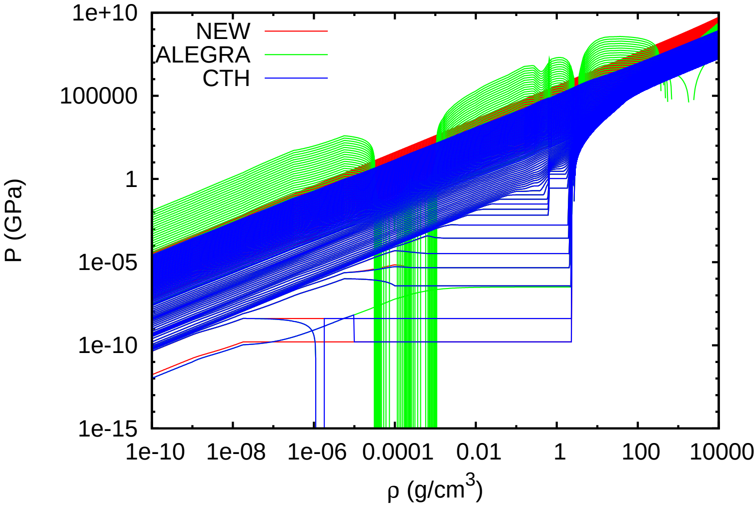
Extrapolation compared – Al 3700 energy



Extrapolation compared – Al 3700 pressure



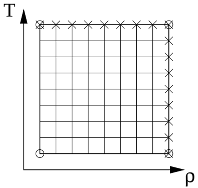
Comprehensive testing setup

Divide table into patches:

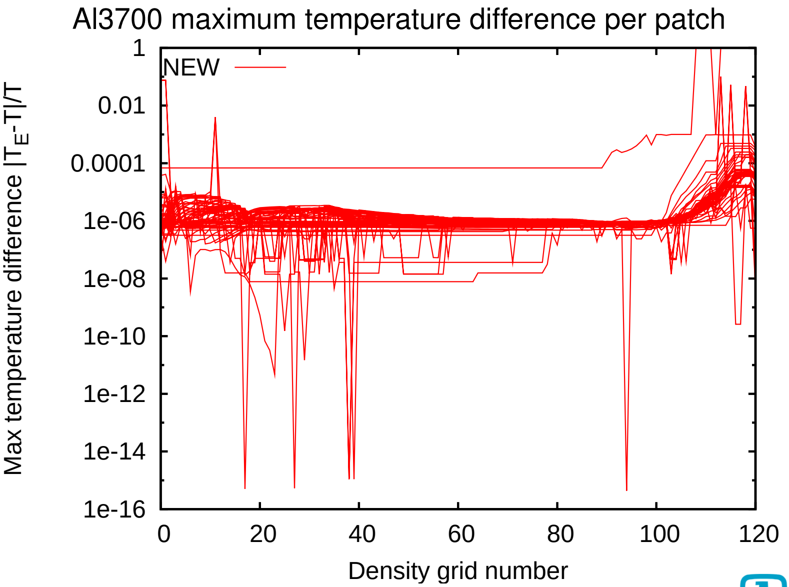
- Each grid point represents a patch
- Composed of current point and those with indices one greater
- Points on the top/right are extrapolation patches

Test each patch:

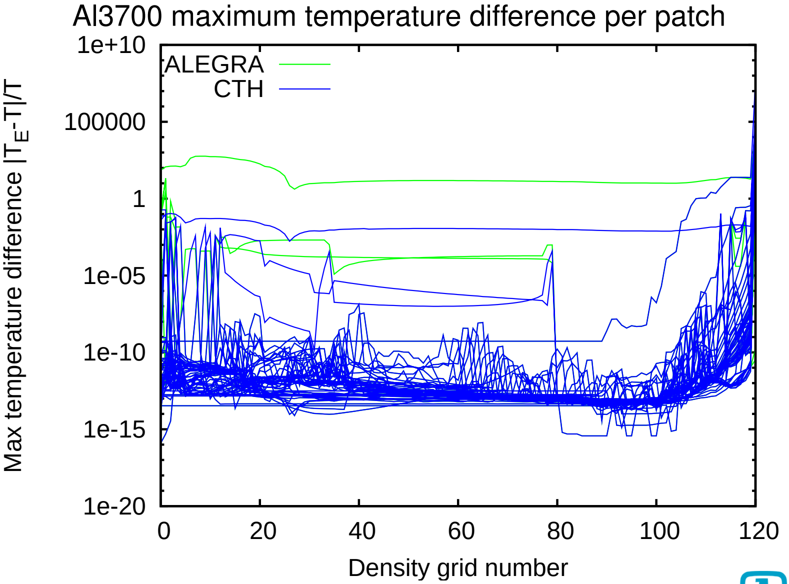
- Lay out a 100x100 uniform grid in ρ and T
  - Extrapolation patches use $1/\rho$ and/or $1/T$
  - Set evaluation points at all grid intersections
- Run the EOS drivers at all points
  - Run the temperature driver first
  - Run the energy driver using the resultant energy
- Check for interpolation problems on each patch
  - Clipping of $\frac{dP}{d\rho}$ and $\frac{dE}{dT}$
  - Convergence of both drivers
  - Consistency between drivers



Consistency of new driver



Consistency of old drivers



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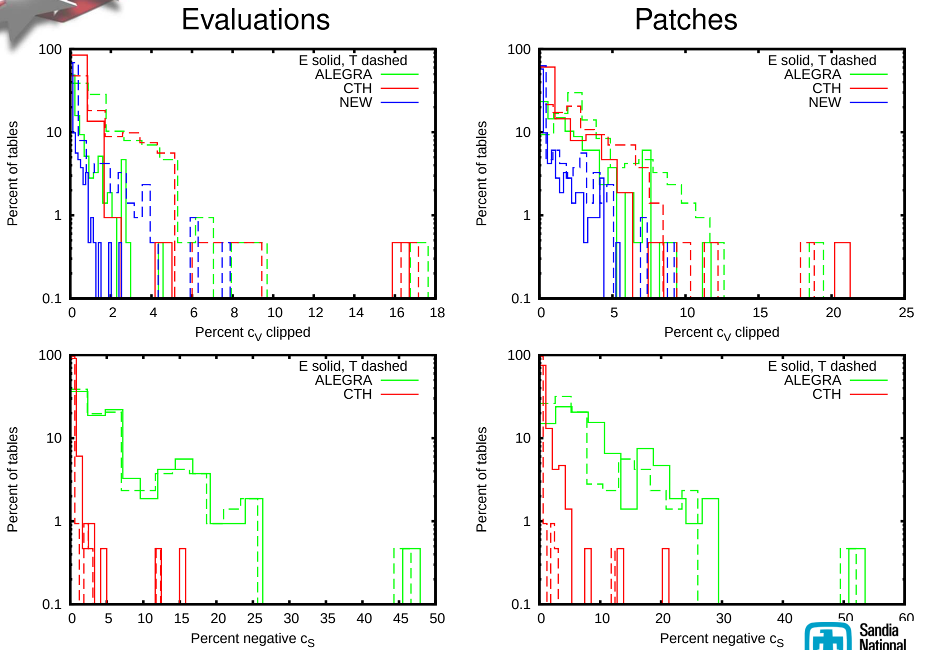
Convergence tests



Simple speed tests

- Percent differences to ALEGRA driver times
- N is the vector size passed to the temperature (T) or energy (E) driver
- Run on Al 3700 table with 60-100 million EOS evaluations

Constant temperature sweep:

	CTH		NEW	
N	T	E	T	E
1	6.0	5.6	9.5	11.6
32	4.7	4.1	3.6	9.0
64	5.6	4.0	6.8	10.7

Random ρ and T:

	CTH		NEW	
N	T	E	T	E
1	6.1	24.5	-2.1	6.9
16	5.3	29.1	0.0	17.3
32	5.1	28.9	-0.9	18.8
64	4.9	28.9	0.2	20.8

Sound speed behavior

$$c_S = \sqrt{\frac{dP}{d\rho} + \frac{T}{\rho^2}\left(\frac{dP}{dT}\right)^2 / \frac{dE}{dT}}$$

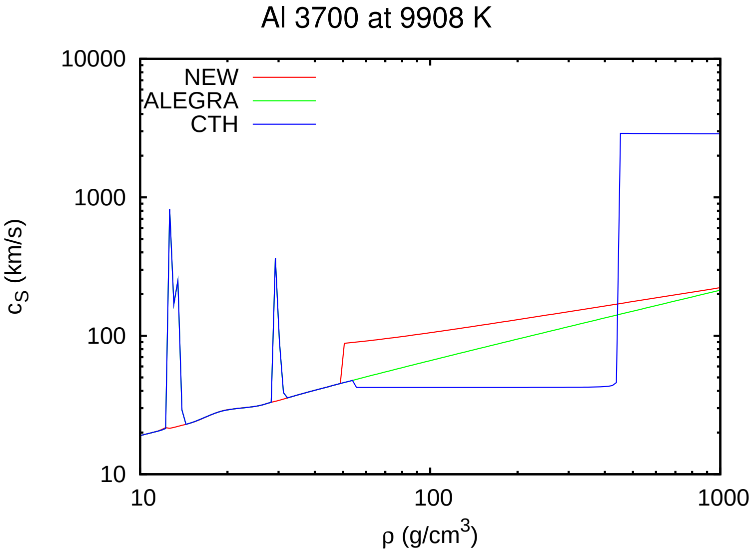
Old:

- negative $\frac{dP}{d\rho}$ clipped at zero, $\frac{dE}{dT}$ at $c_{V,min}$
- ensures real, but abnormally large, c_S
- If in unphysical tension ($\rho < \rho_{min}$, $P < 0$) CTH sets to one and ALEGRA recomputes
- If SESESV fails to converge ALEGRA recomputes c_S

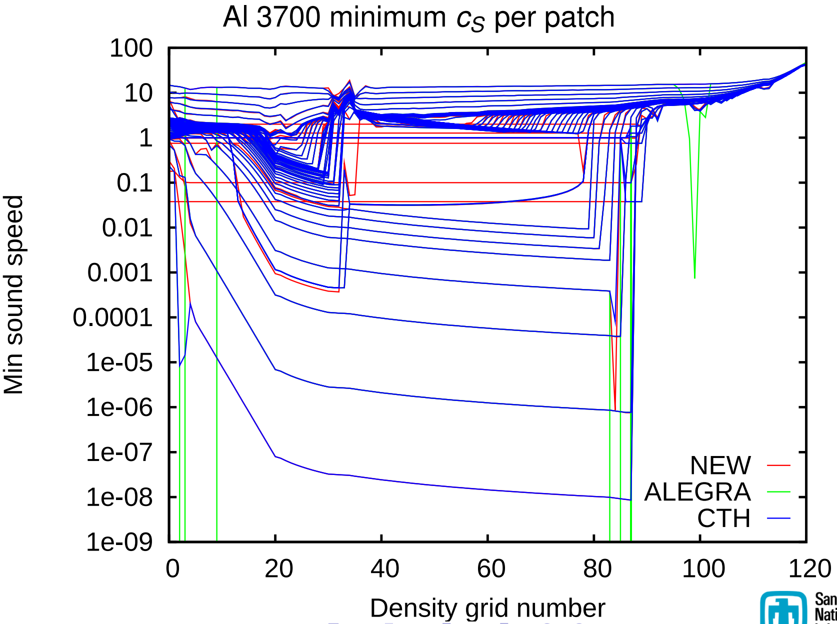
New:

- If $\frac{dP}{d\rho} < 0$ and $P > 0$ then $\frac{dP}{d\rho} = -\frac{dP}{d\rho}$
- If $\frac{dE}{dT} < 0$ then $\frac{dE}{dT} = -\frac{dE}{dT}$
- Clips are subsequently applied
- If $\frac{dP}{d\rho} = 0$ and $\frac{dP}{dT} = 0$ then $c_S = \sqrt{T\frac{dE}{dT}}$
- Works on the assumption that if the derivative is negative, its magnitude, rather than the floor, better approximates a value that will give a continuous sound speed

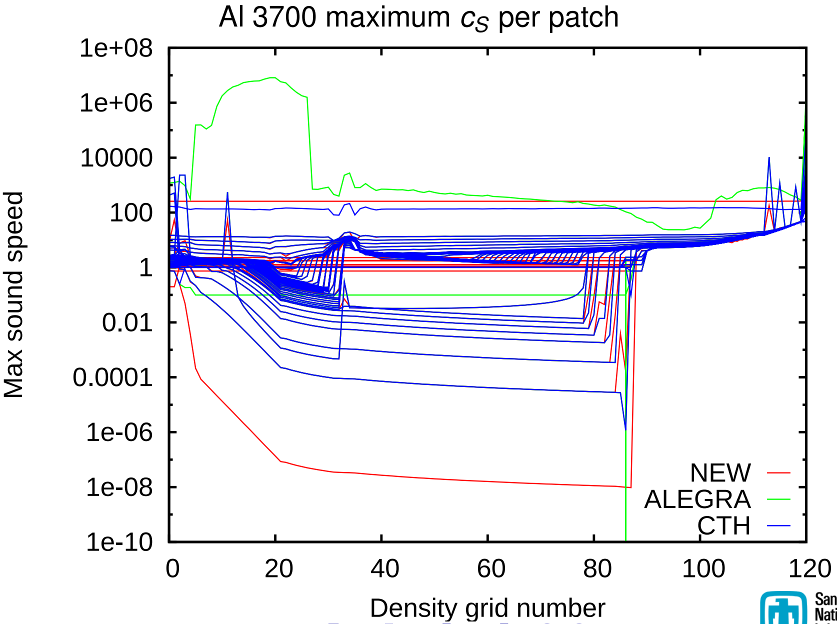
New sound speed behavior



Overall sound speed behavior



Overall sound speed behavior



New temperature clip options for keos sesame

Old behavior:

- CLIP – clip high and low temperatures
- CLIP{HI,LO} – clip either high or low temperatures
- all values relative to edge of table
- defaults: no clipping and no message output

New behavior:

- CLIPH (CLIPHI) – high T clip behaving like old CLIPHI
- CLIPL (CLIP) – low T clip for $\rho > \rho_{min}$
- CLIPT (CLIPLO) – low T clip for $\rho < \rho_{min}$
- CLIPH relative to table edge, CLIP{L,T} absolute
- defaults: CLIPL = 0.01 K, CLIPH off, CLIPT = T of first isotherm with $P > 0$ at lowest $\rho > 0$, no message output
- If (CLIPL > CLIPT) then CLIPT = CLIPL
- A negative clip value still suppresses message output

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