LA-UR-20-30467

Title: Sound Speed Calculations in EOSPAC6

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Sound Speed Comparisons in EOSPAC6

Daniel Sheppard

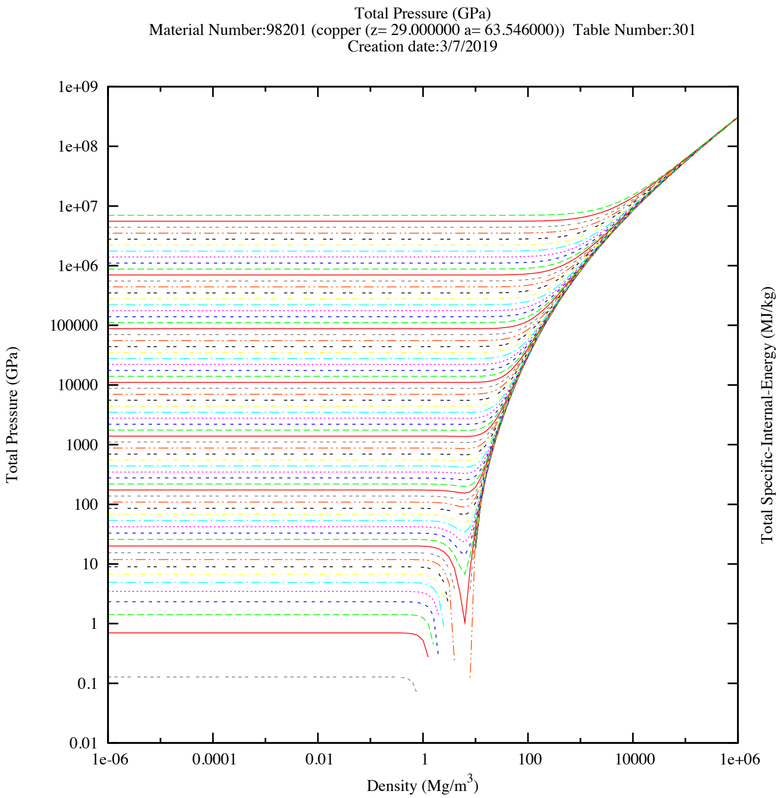
Are all thermodynamic relations created equal?

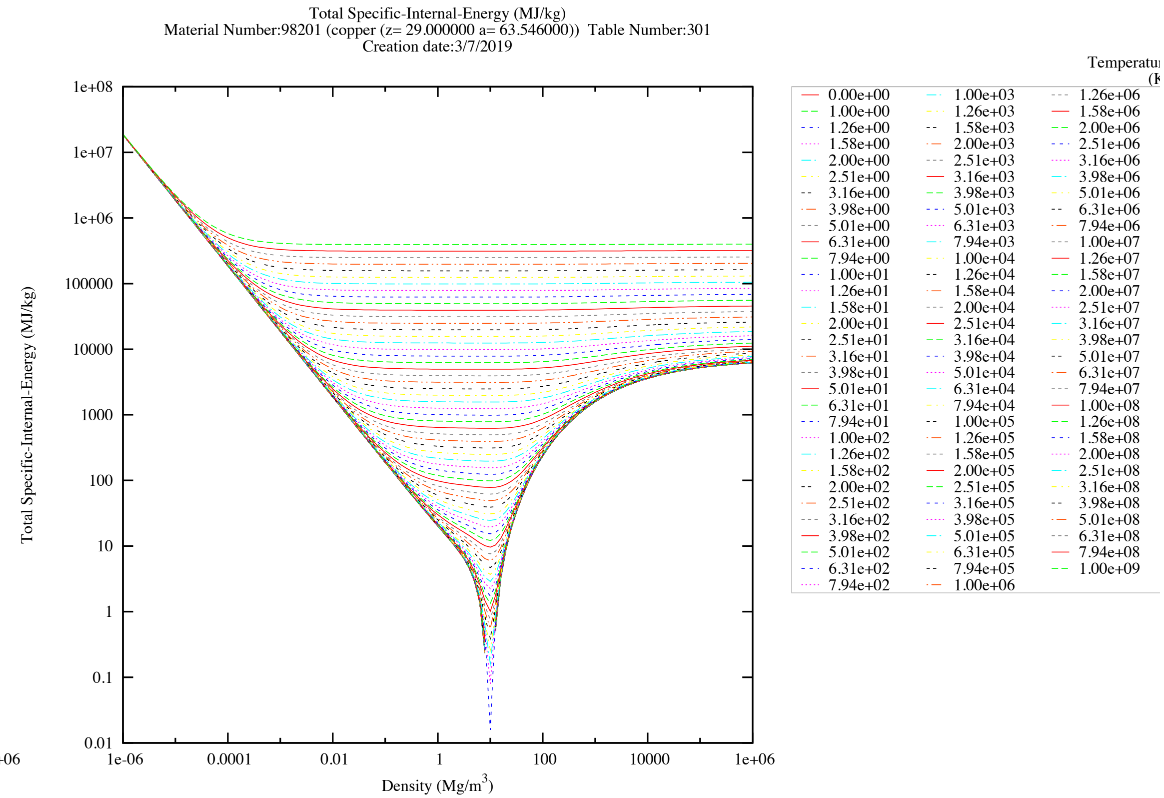
Black: direct interpolation
Green: inverted with respect to second variable
Blue: constructed from two other tables

eospac6 calls	sound-speed derivation	eq. label
• eos_Pt_DT, eos_Ut_DT	$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_T + \frac{T}{\rho^2 \left(\frac{\partial U}{\partial T}\right)_\rho} \left(\frac{\partial P}{\partial T}\right)_\rho^2$	(1) Menikoff
• eos_Pt_DUt	$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_U + \frac{P}{\rho^2} \left(\frac{\partial P}{\partial U}\right)_\rho$	(2) FLAG
• eos_T_DUt, eos_Pt_DT	$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_T + \left(\frac{\partial P}{\partial T}\right)_\rho \left[\left(\frac{\partial T}{\partial \rho}\right)_U + \frac{P}{\rho^2} \left(\frac{\partial T}{\partial U}\right)_\rho\right]$	(3) Peterson
• eos_Pt_DSt	$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_S$	(4) entropy
• eos_St_DPt	$c^2 = \frac{-\left(\frac{\partial S}{\partial \rho}\right)_P}{\left(\frac{\partial S}{\partial P}\right)_\rho}$	(5) entropy2

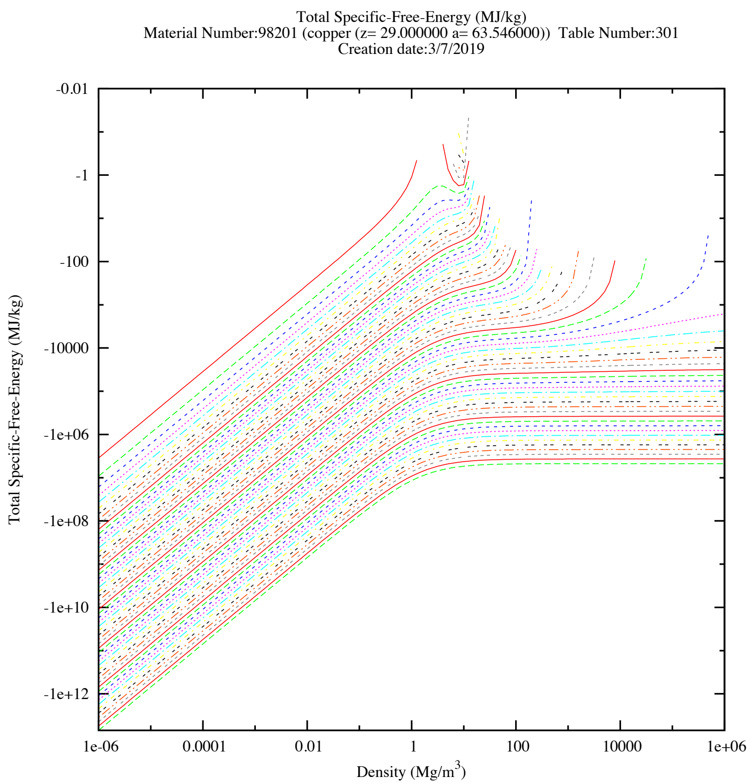
Test case 1: Analytic copper: MATID = -8201

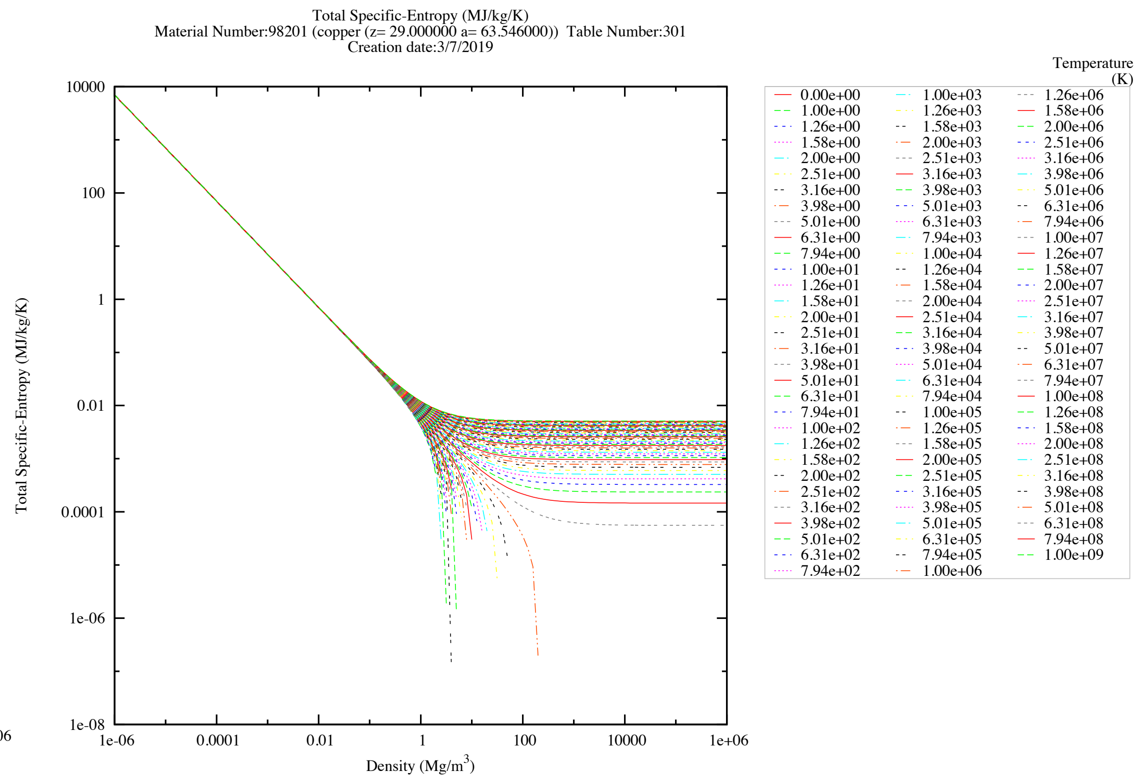
Pressure/Density and Energy Density



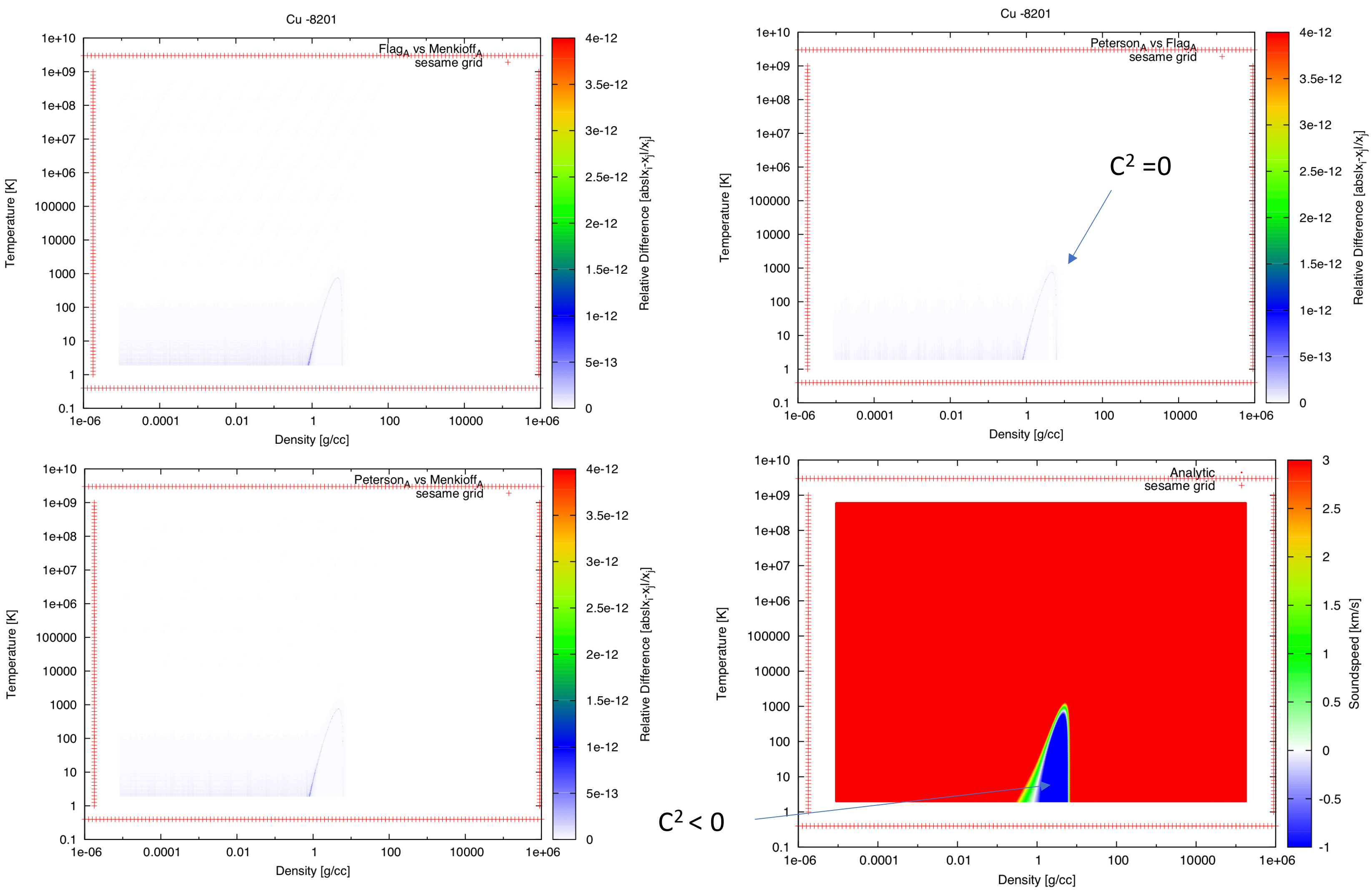


Helmholtz/Density and Entropy/Density

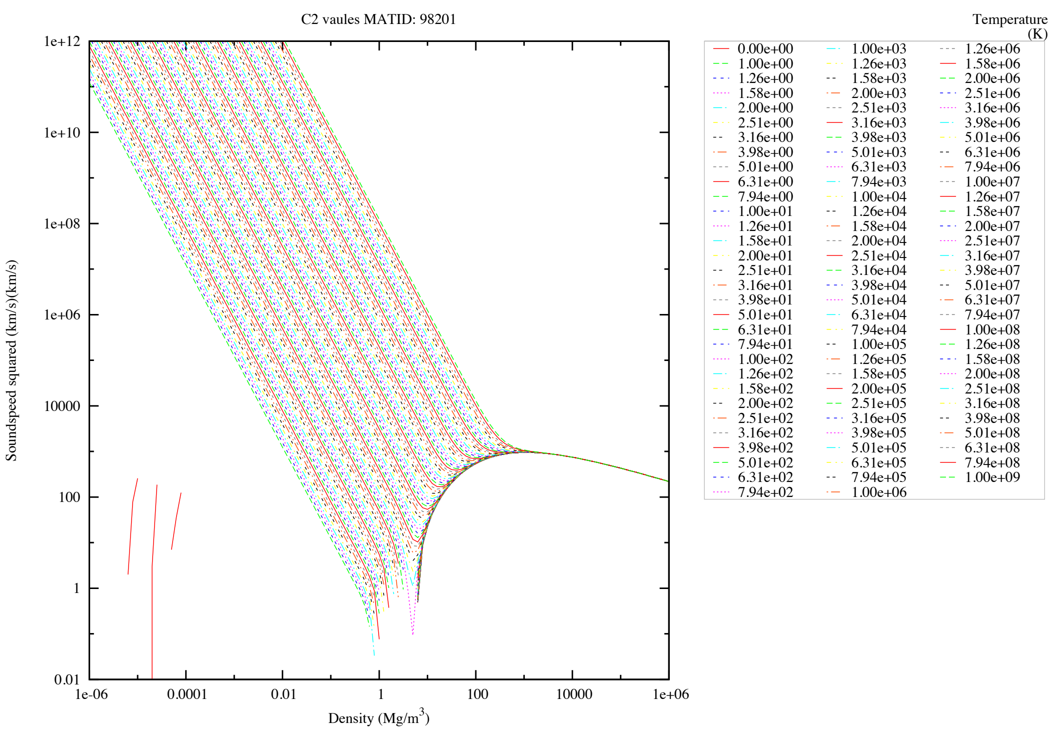


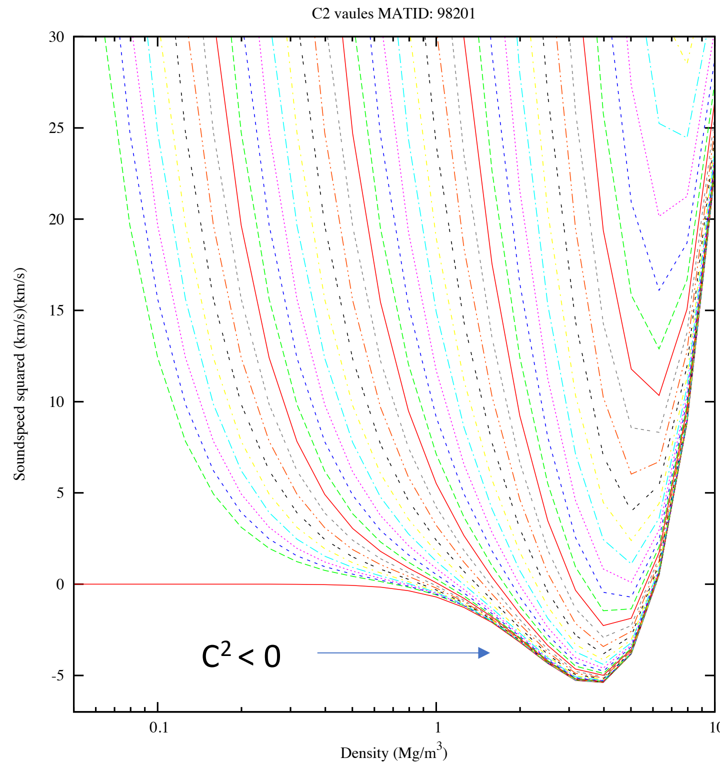


Analytic comparisons



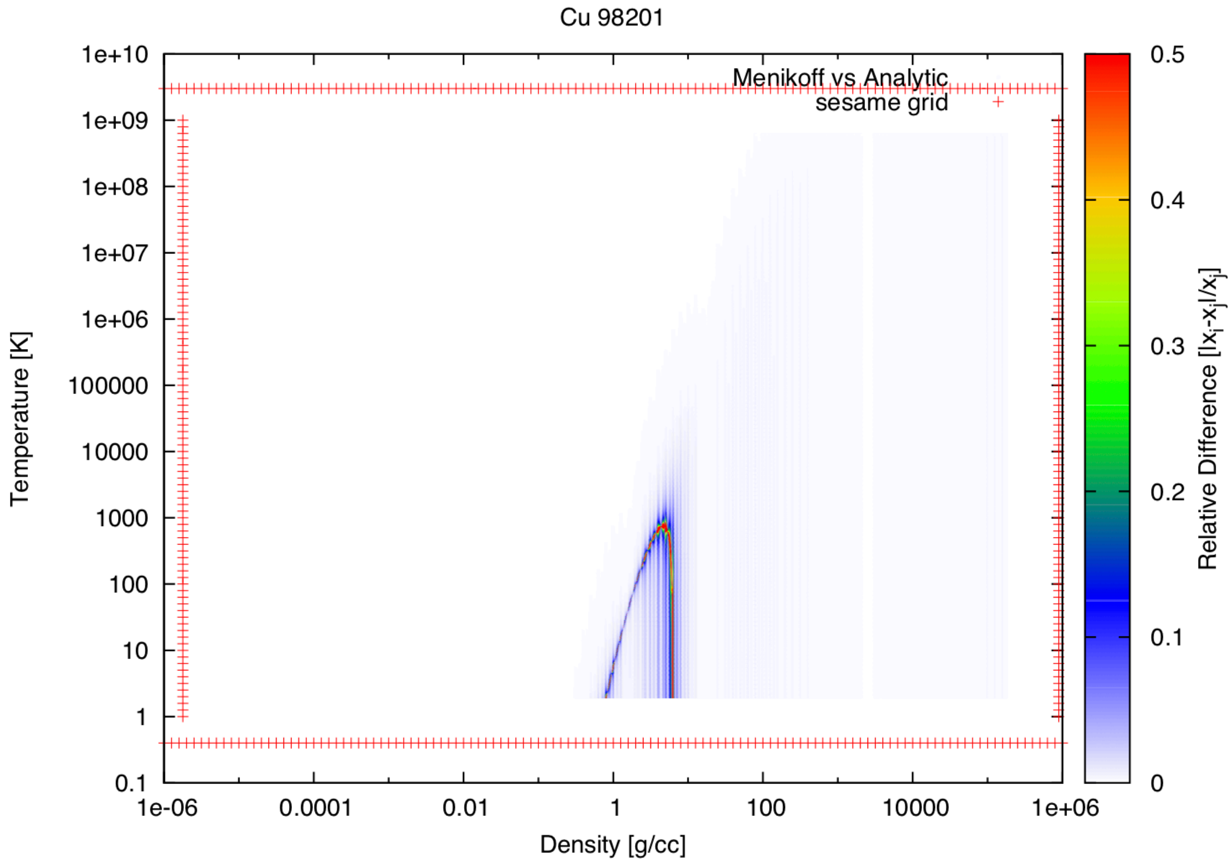
C^2 vs Density



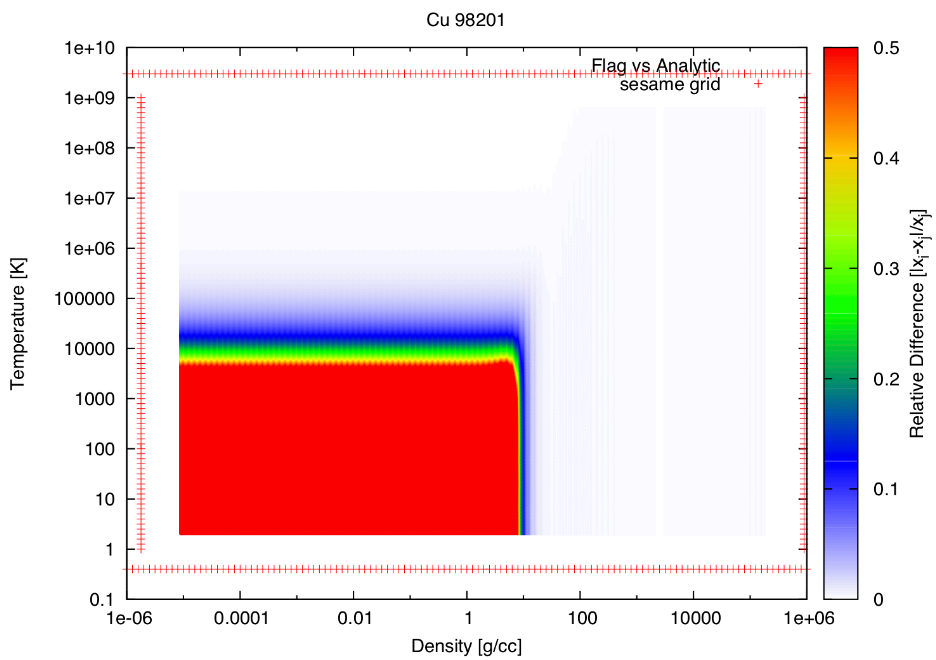


Menikoff does the best in expansion

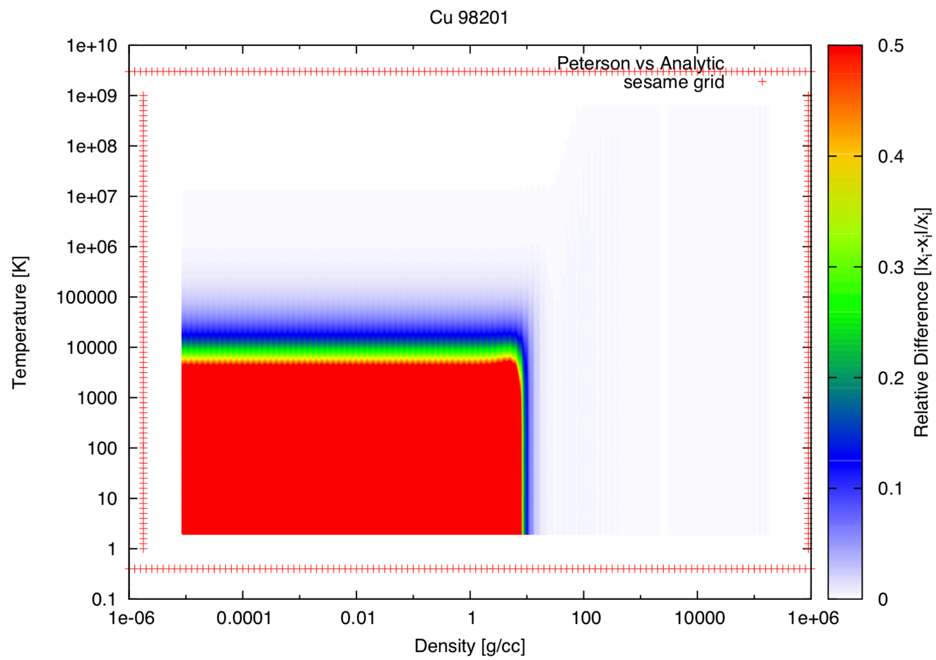
$$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_T + \frac{T}{\rho^2 \left(\frac{\partial U}{\partial T}\right)_\rho}\left(\frac{\partial P}{\partial T}\right)_\rho^2$$



Flag and Peterson: bad in expansion?



$$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_U + \frac{P}{\rho^2}\left(\frac{\partial P}{\partial U}\right)_\rho$$



$$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_T + \left(\frac{\partial P}{\partial T}\right)_\rho \left[\left(\frac{\partial T}{\partial \rho}\right)_U + \frac{P}{\rho^2}\left(\frac{\partial T}{\partial U}\right)_\rho\right]$$

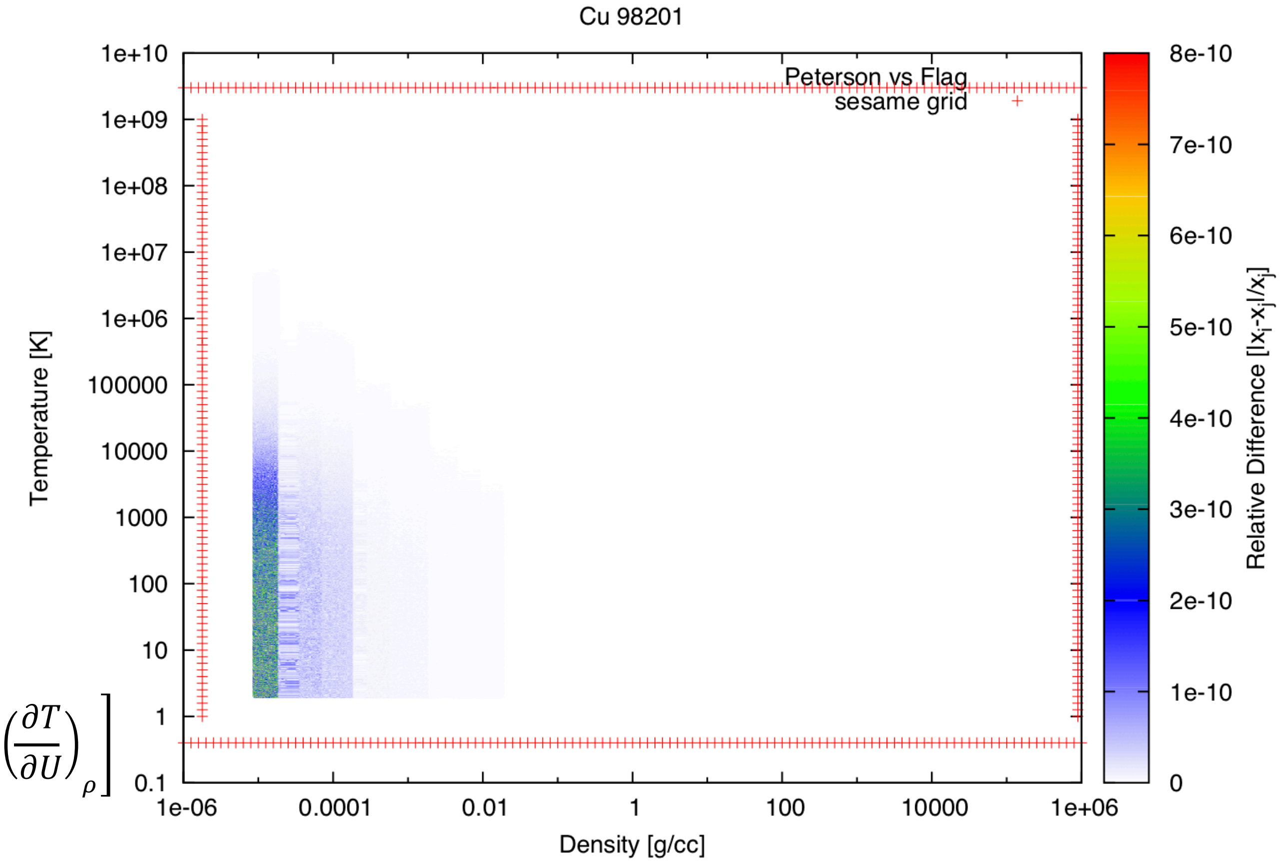
Peterson vs Flag are numerically consistent

FLAG

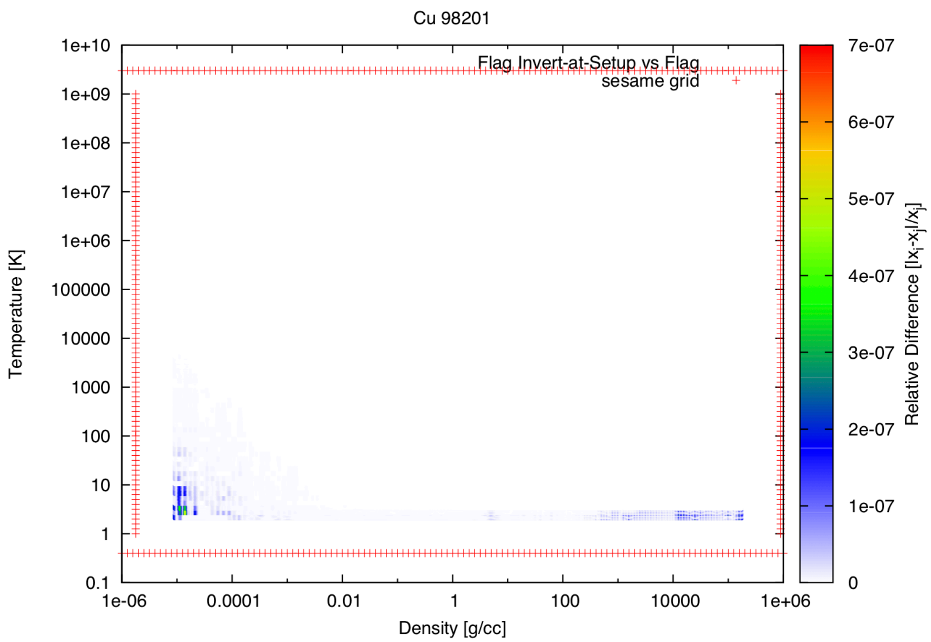
$$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_U + \frac{P}{\rho^2}\left(\frac{\partial P}{\partial U}\right)_\rho$$

Peterson

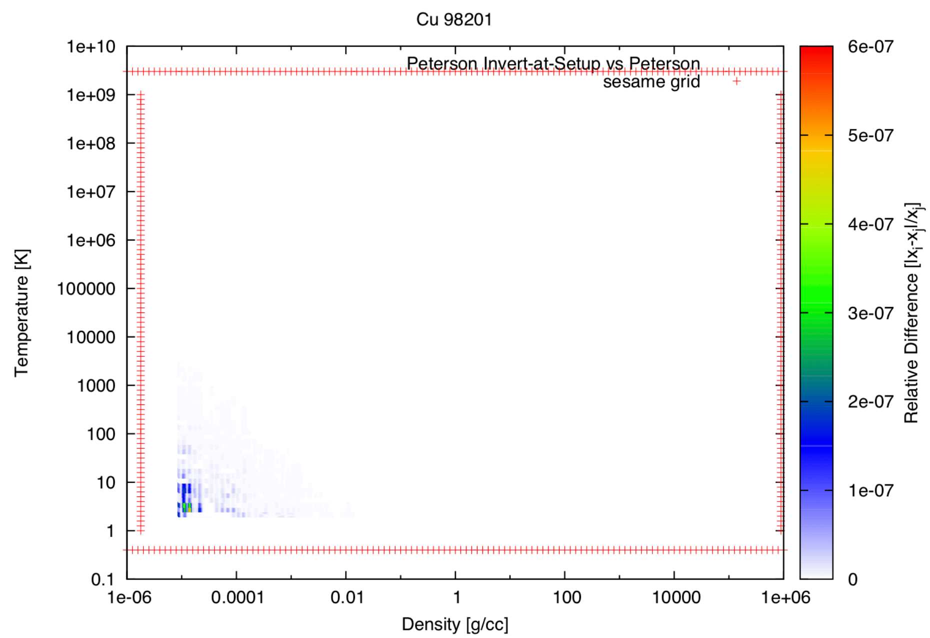
$$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_T + \left(\frac{\partial P}{\partial T}\right)_\rho \left[\left(\frac{\partial T}{\partial \rho}\right)_U + \frac{P}{\rho^2}\left(\frac{\partial T}{\partial U}\right)_\rho\right]$$



Default interpolation vs. Invert_At_Setup

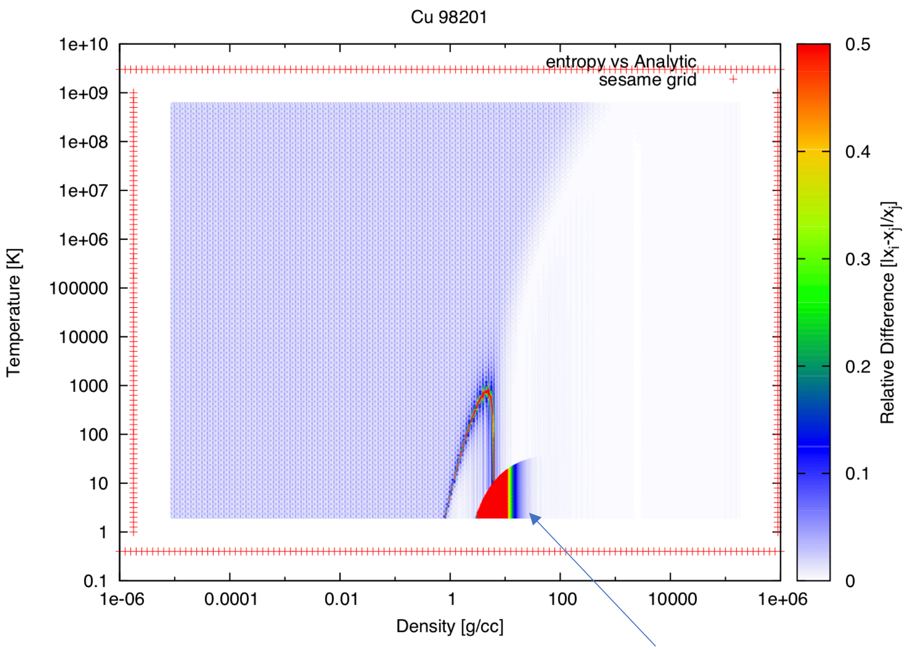


$$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_U + \frac{P}{\rho^2}\left(\frac{\partial P}{\partial U}\right)_\rho$$

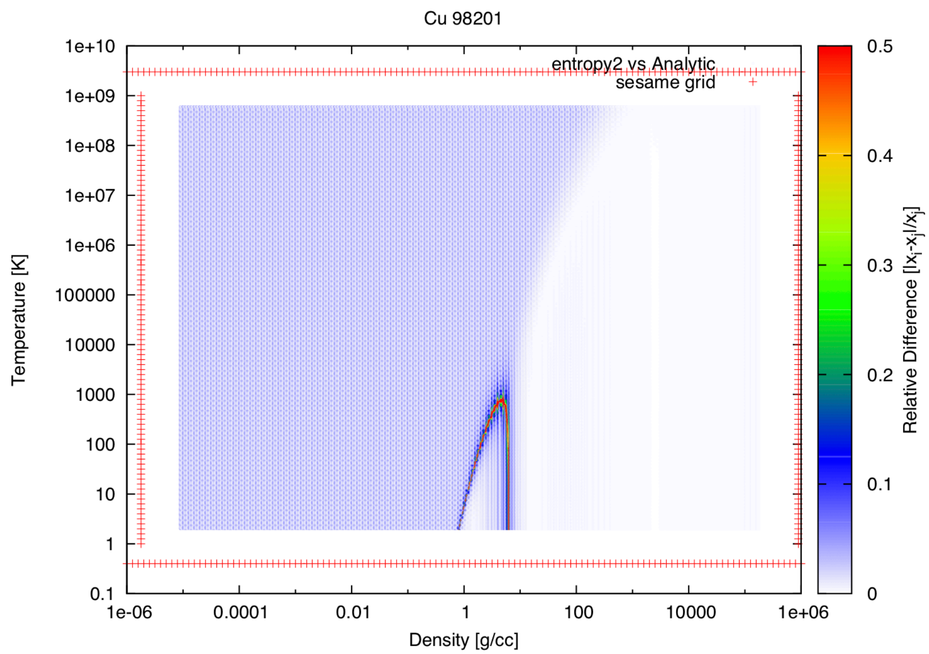


$$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_T + \left(\frac{\partial P}{\partial T}\right)_\rho \left[\left(\frac{\partial T}{\partial \rho}\right)_U + \frac{P}{\rho^2}\left(\frac{\partial T}{\partial U}\right)_\rho\right]$$

Auto generated entropy tables for C^2

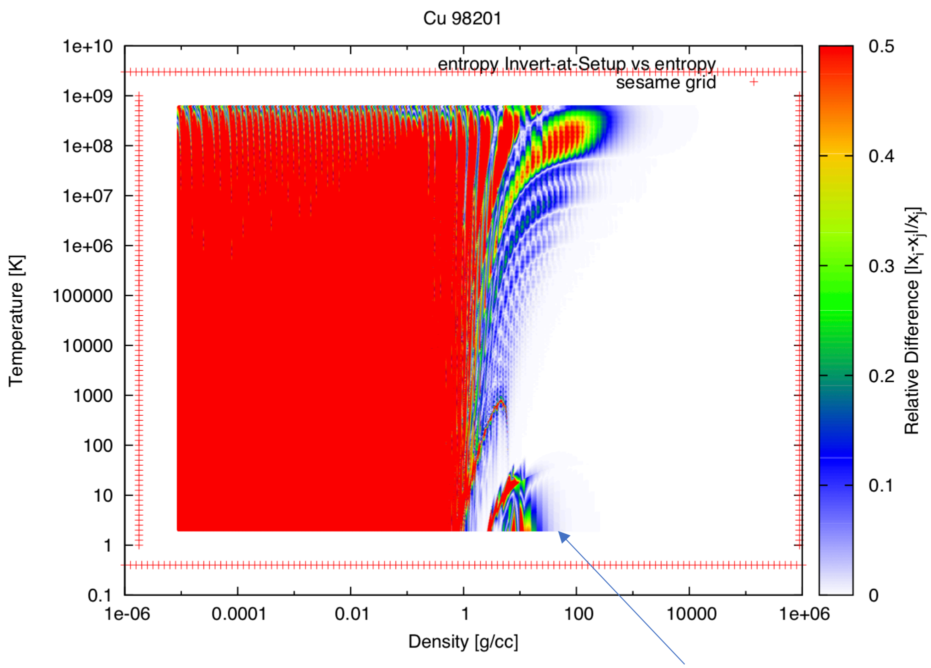


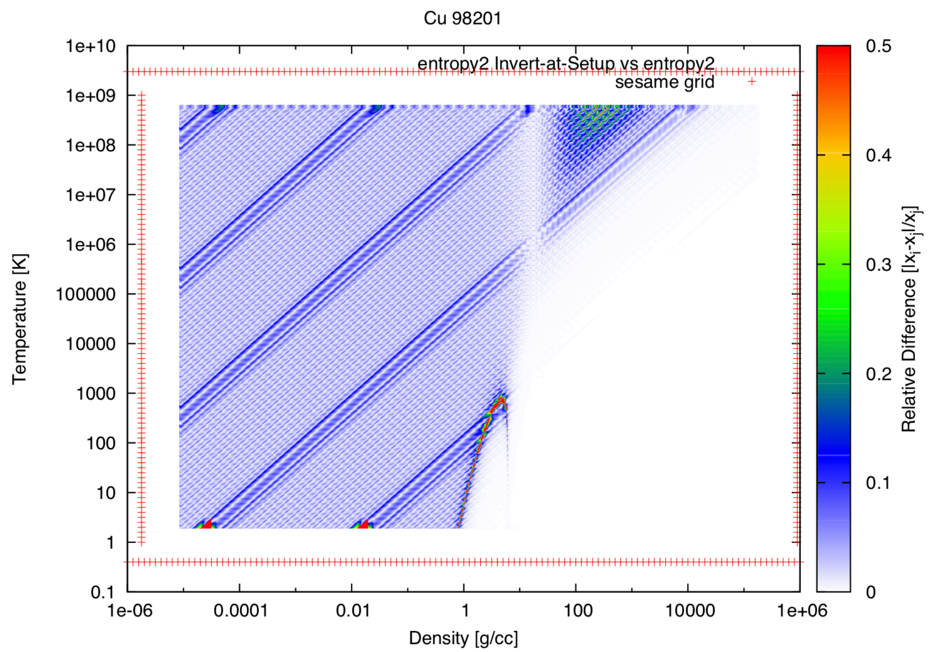
$$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_S$$



$$c^2 = \frac{-\left(\frac{\partial S}{\partial \rho}\right)_P}{\left(\frac{\partial S}{\partial P}\right)_\rho}$$

Invert_At_Setup entropy tables for C^2



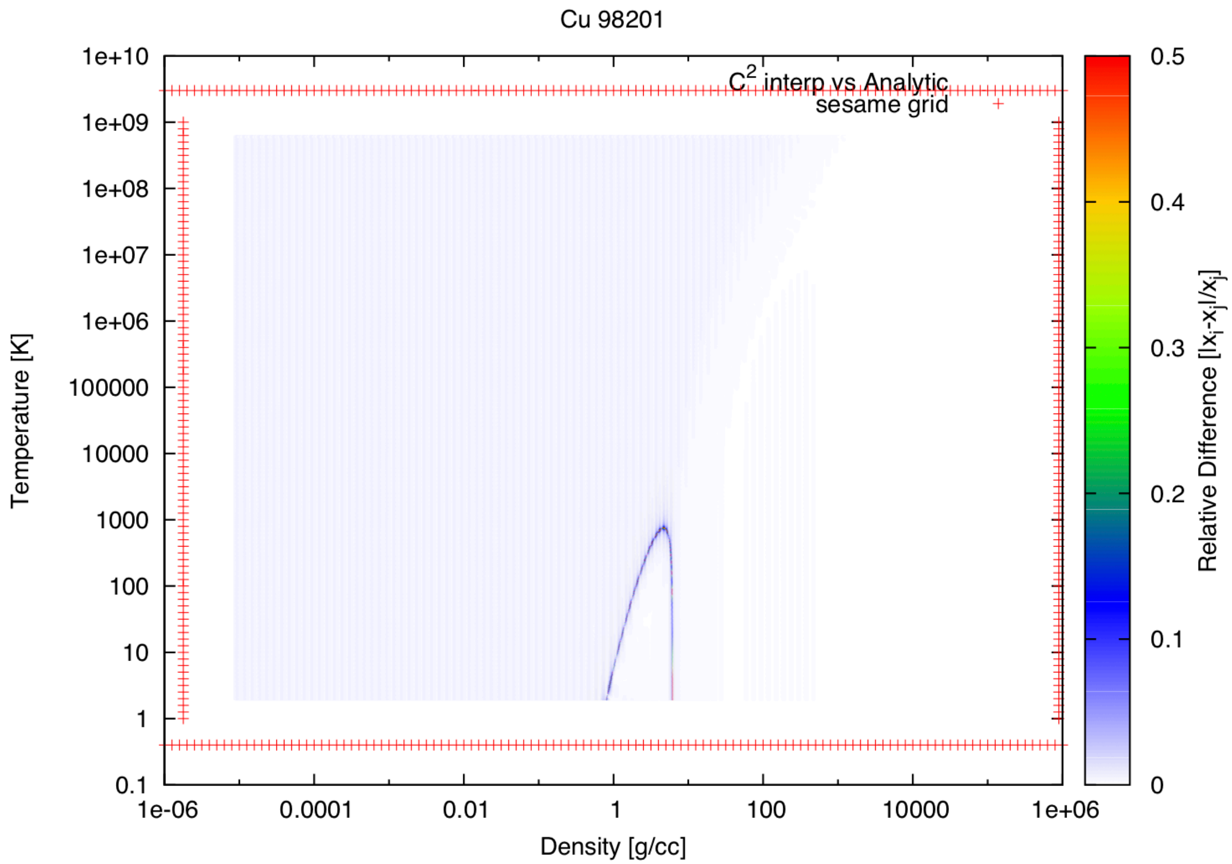


Extrapolation

$$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_S$$

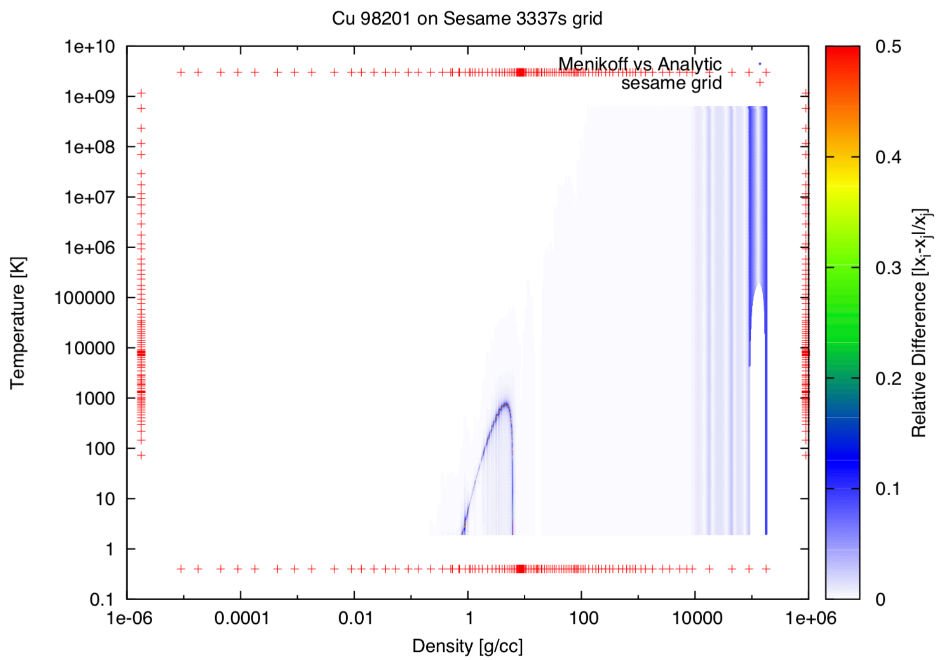
$$c^2 = \frac{-\left(\frac{\partial S}{\partial \rho}\right)_P}{\left(\frac{\partial S}{\partial P}\right)_\rho}$$

Direct Tabulation of C^2 in 300 style table

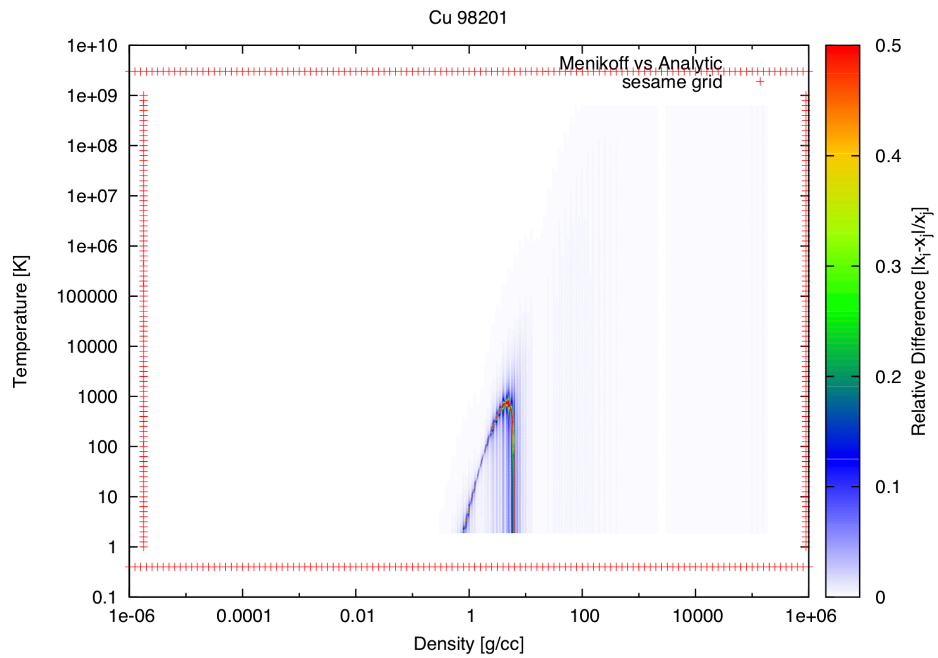


Menikoff

$$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_T + \frac{T}{\rho^2 \left(\frac{\partial U}{\partial T}\right)_\rho} \left(\frac{\partial P}{\partial T}\right)_\rho^2$$



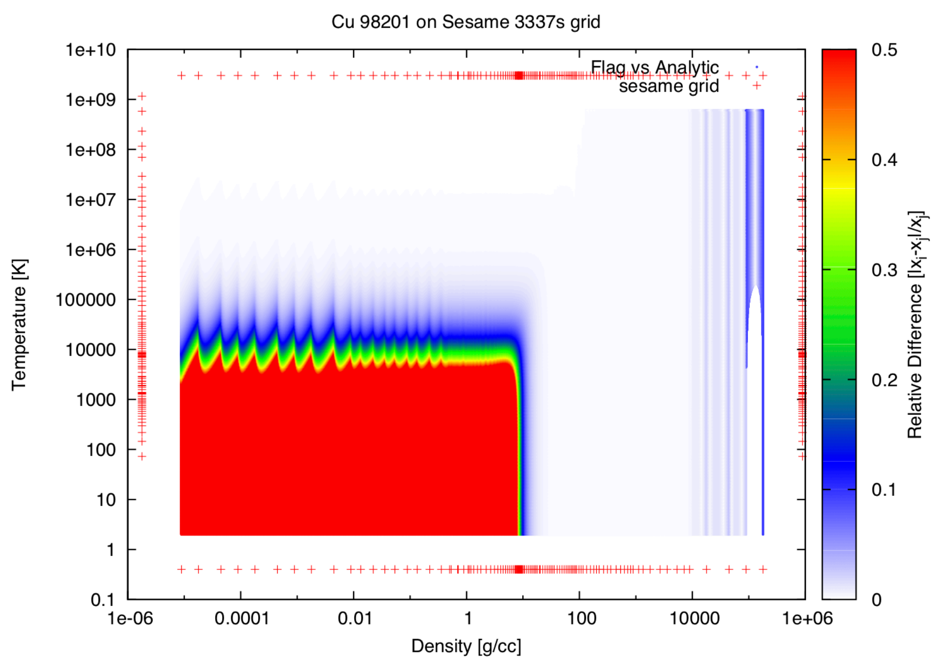
Typical Sesame Grid



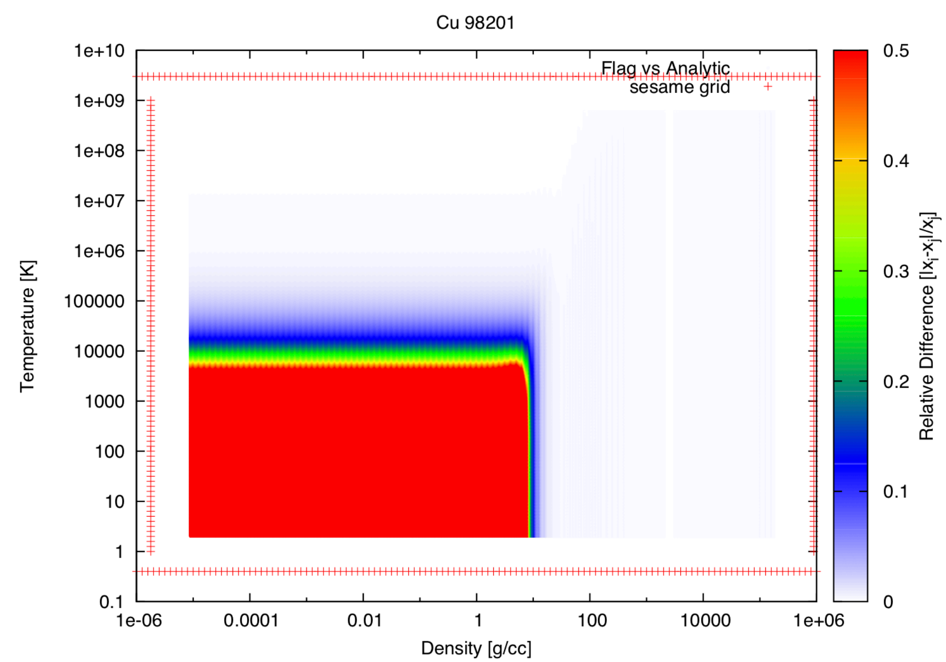
Even log spacing

FLAG

$$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_U + \frac{P}{\rho^2}\left(\frac{\partial P}{\partial U}\right)_\rho$$



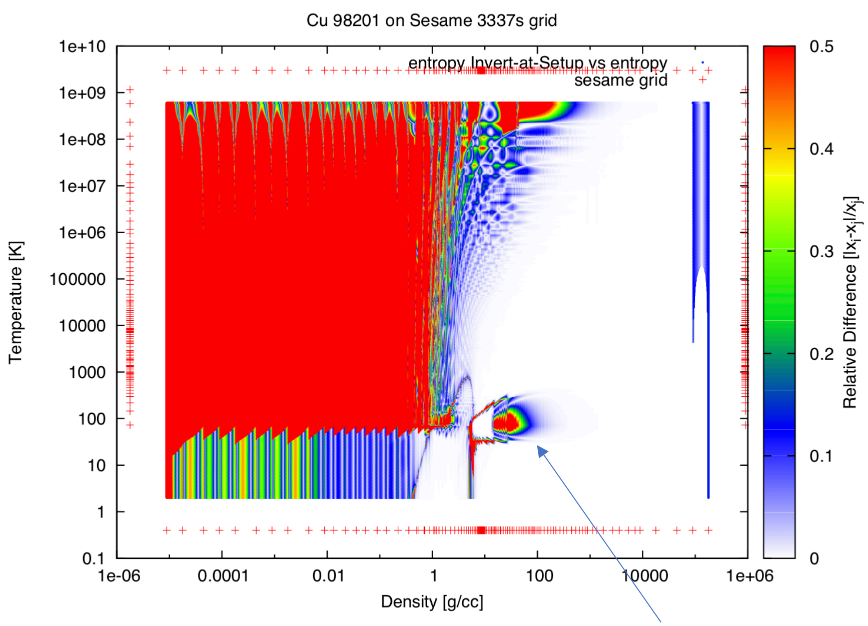
Typical Sesame Grid



Even log spacing

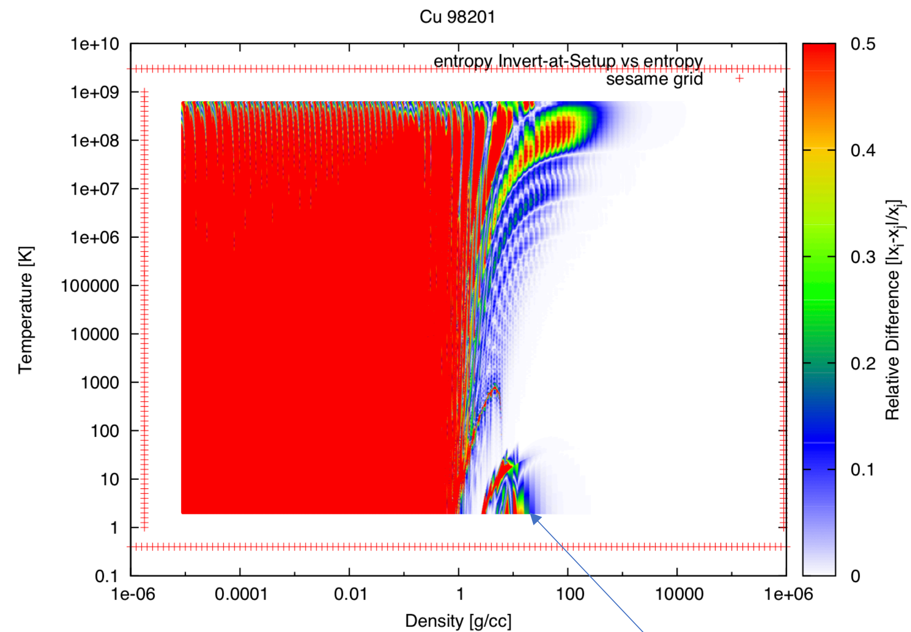
Entropy1 Invert_At_Setup

$$c^2 = \left(\frac{\partial P}{\partial \rho}\right)_S$$



Extrapolation

Typical Sesame Grid

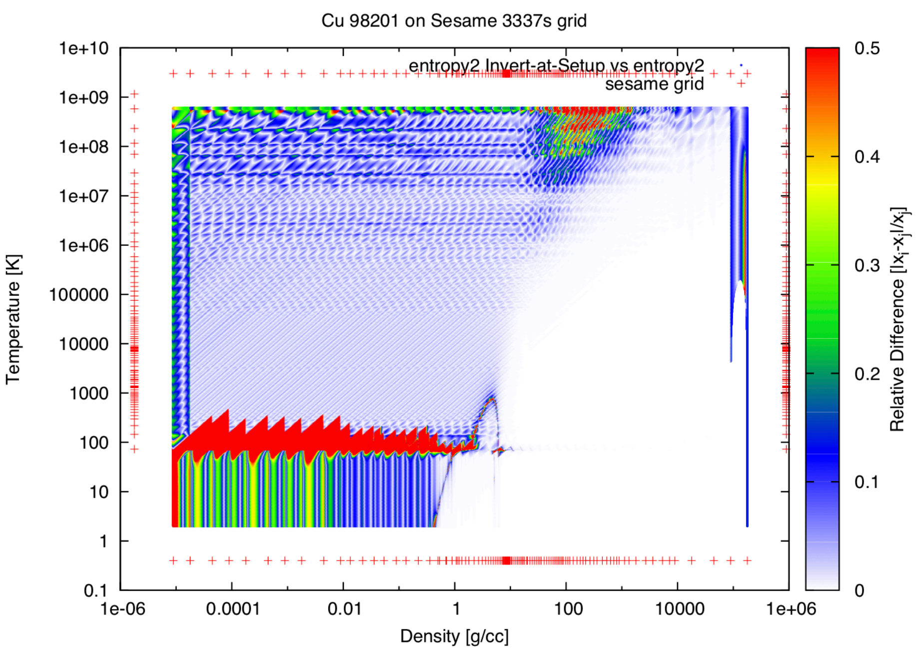


Extrapolation

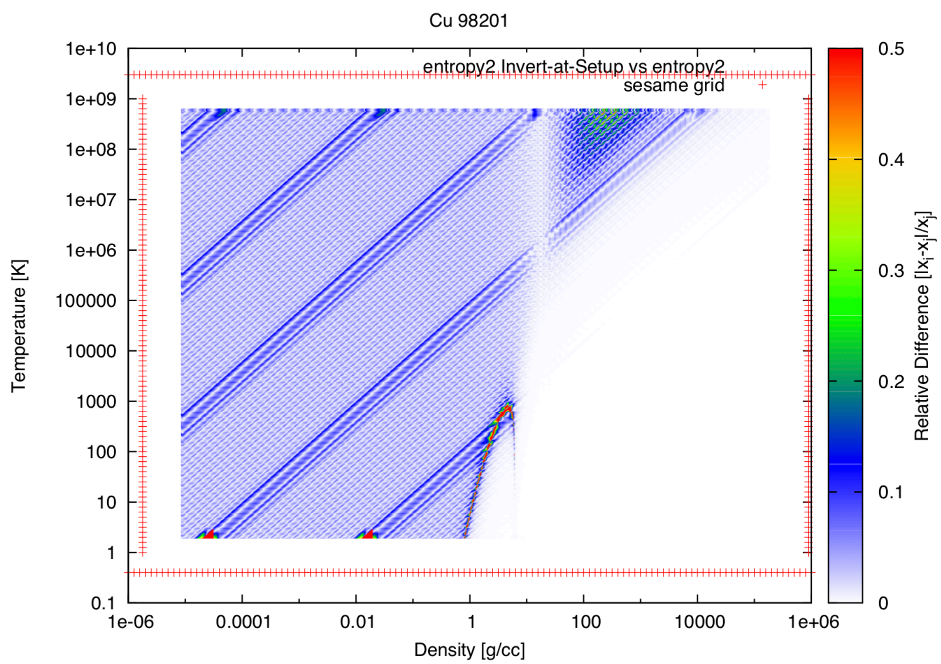
Even log spacing

Entropy2 Invert_At_Setup

$$c^2 = \frac{-\left(\frac{\partial S}{\partial \rho}\right)_P}{\left(\frac{\partial S}{\partial P}\right)_\rho}$$

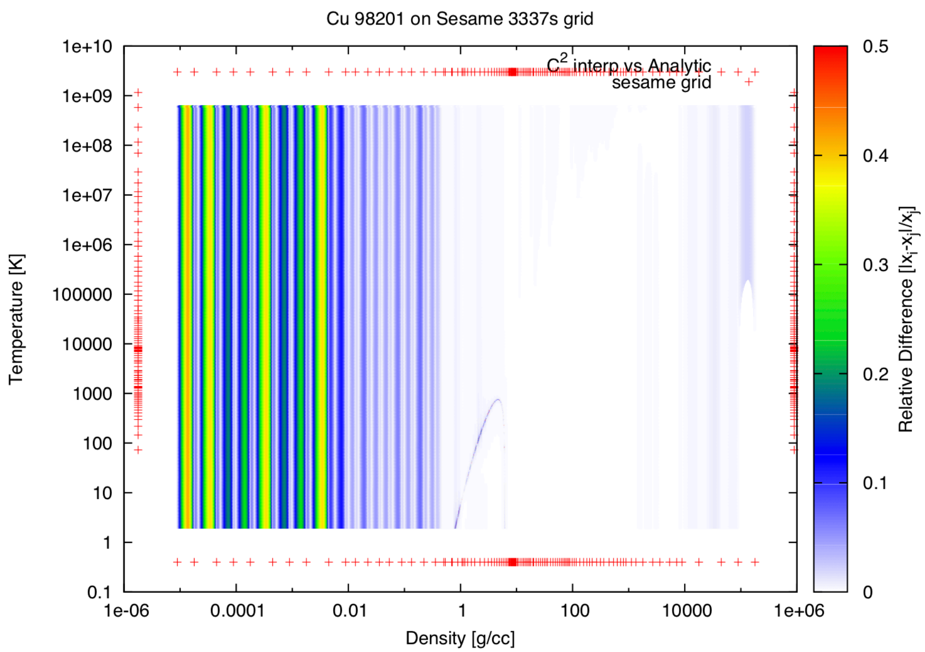


Typical Sesame Grid

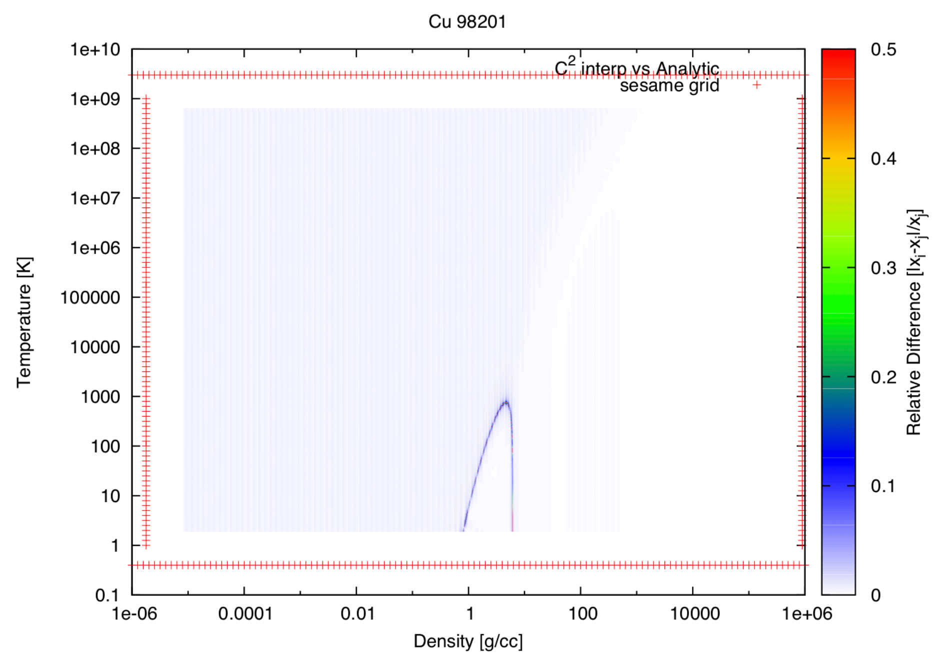


Even log spacing

Direct Tabulation of C^2 in 300 style table

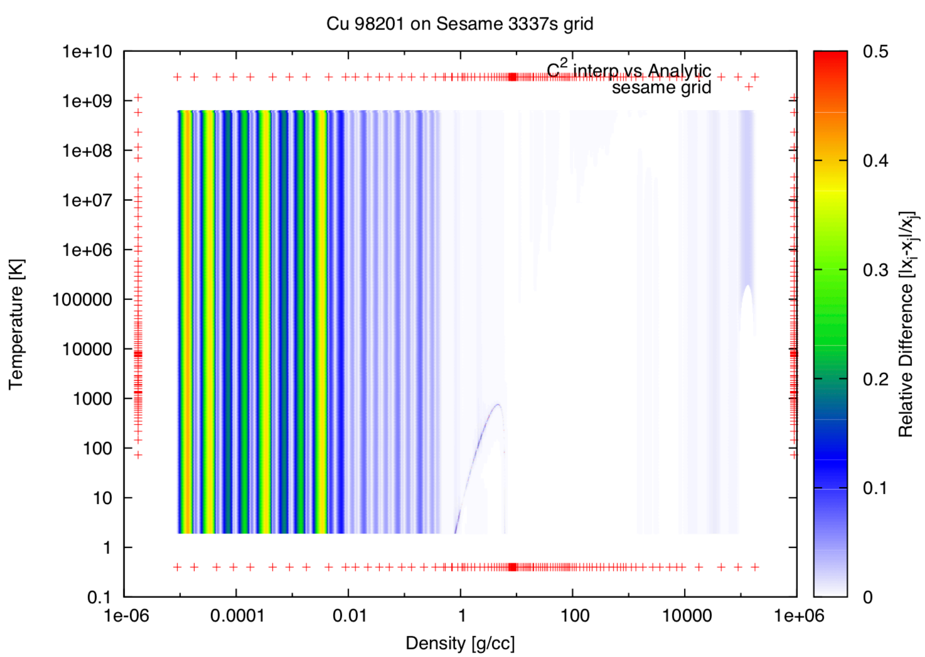


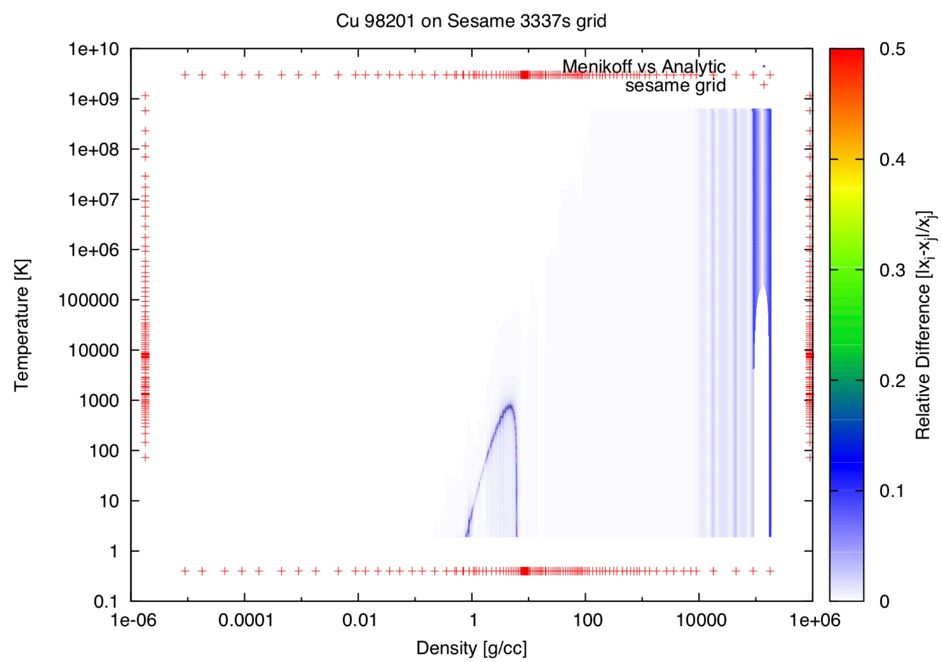
Typical Sesame Grid



Even log spacing

Menikoff vs direct interpolation of C^2





Menikoff vs direct interpolation of C^2