EOS

- Physics of the EOS
- Range of thermodynamical parameters (ρ, T, P, E_{int})
- Metallicity (X, Y, Z)

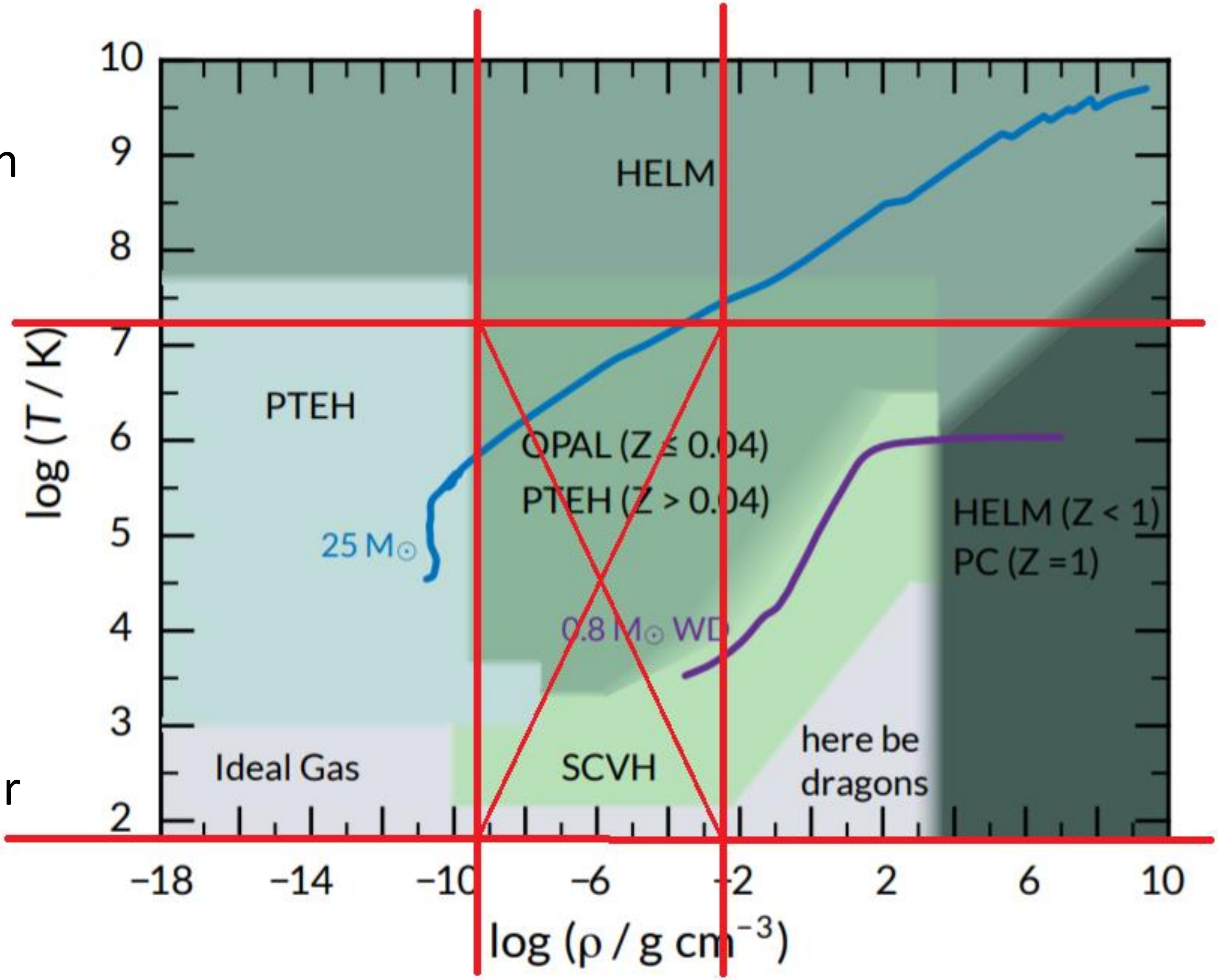
- Current status regarding putting into ASTROBear

Parameters

- Range of parameters in CE run 143
- $-9.2 < \log\rho < -2.3$
- $0.5 < \log T < 7.3$
- $1.3 < \log E^{(1)} < 13.1$
- $1.1 < \log P < 12.9$

$^{(1)}$ From VISIT, per volume?

- Other simulations have similar ranges?



Ideal Gas

- Particles are classical and in motion.
- The particles have negligible volume.
- The particles don't interact. There are no attractive or repulsive forces between them.
- The average translational kinetic energy of the gas particles is proportional to temperature.

Two ways to calculate EOS

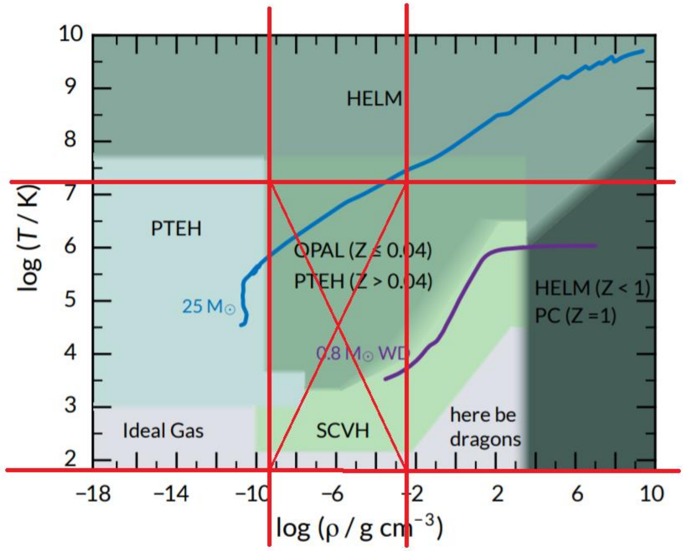
- Physical Picture (OPAL)
  - Treat gas as individual particles
  - Start from Grand Canonical Ensemble: assume a system in thermodynamical equilibrium with a heat reservoir; but allow <u>heat exchange</u> and <u>particle exchange</u>

  - Physical but computationally expensive

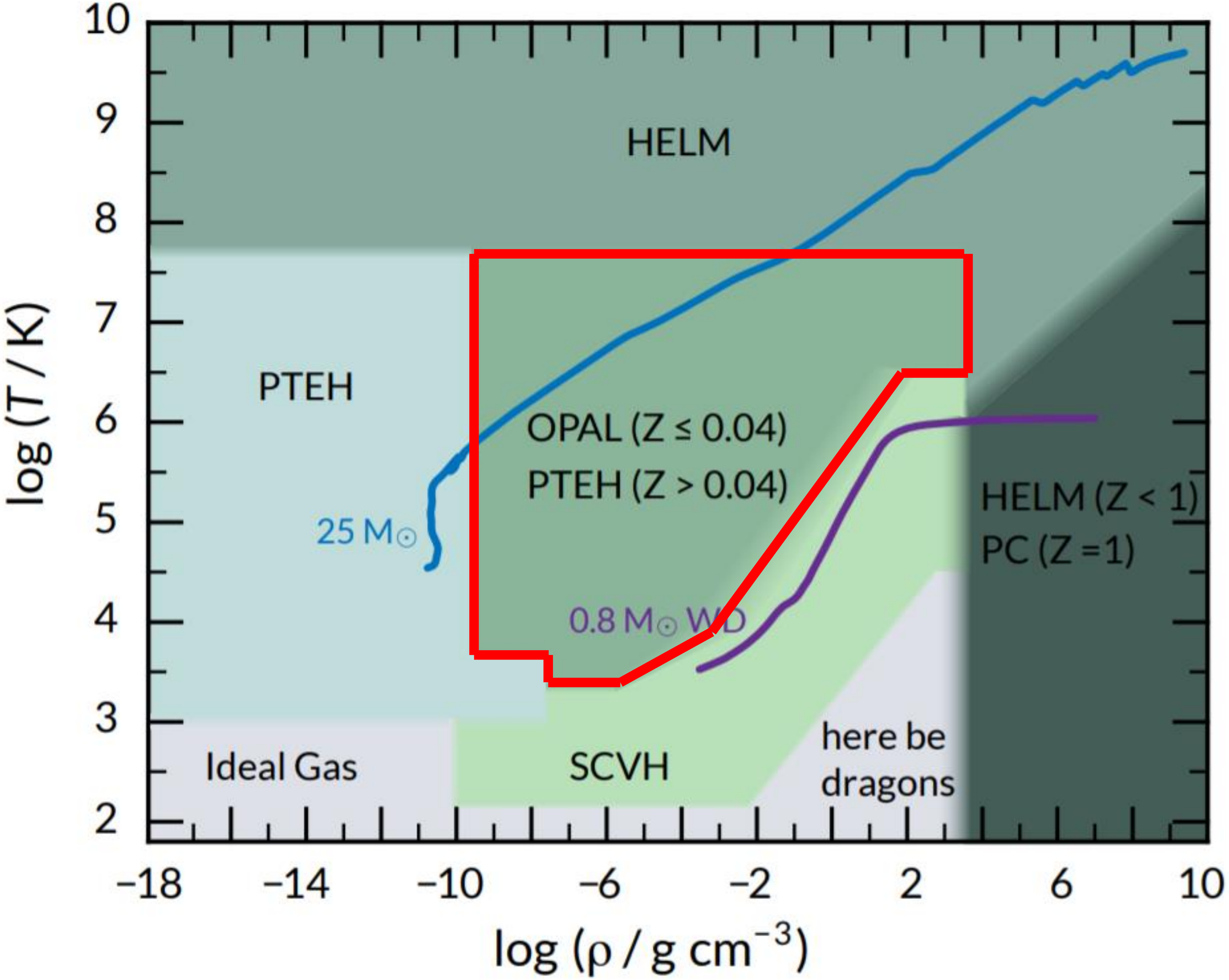
- Chemical picture (all others)
  - Consider atoms and molecules retain a definite identity and interact through pair potentials
  - Solve the quantum problem first, then consider everything as "states''

  - Drawback: when pressure allows pressure-ionization, pair potential becomes meaningless

OPAL



HELM
PTEH
OPAL (Z ≤ 0.04)
PTEH (Z > 0.04)
25 M⊙
0.8 M⊙ WD
HELM (Z < 1)
PC (Z = 1)
Ideal Gas
SCVH
here be dragons
log (T / K)
log (ρ / g cm^{-3})



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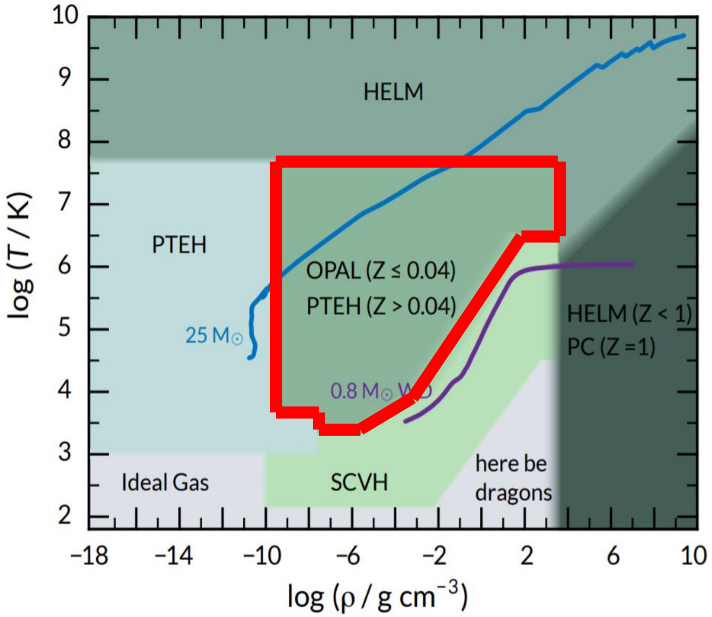
OPAL EOS

- Considers …
  - Physical picture
  - Expands pressure into two-body, three-body clusters
  - Non-relativistic Fermi-Dirac electron
  - All stages of ionization and excitation
  - Degenerate coulomb corrections
  - Quantum electron diffraction
  - Pressure ionization
  - Ladder diagram (consider particle size)
- Accuracy to the order $(n_e^2)^{5/2}$

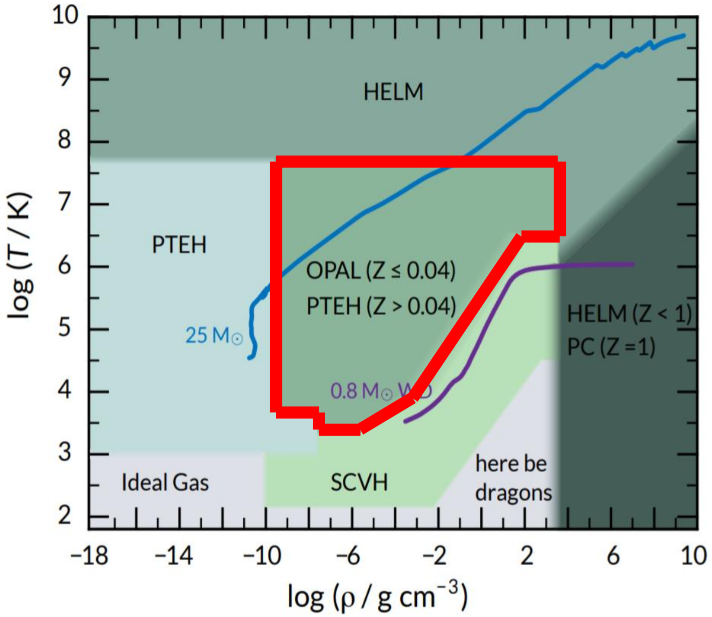


OPAL EOS

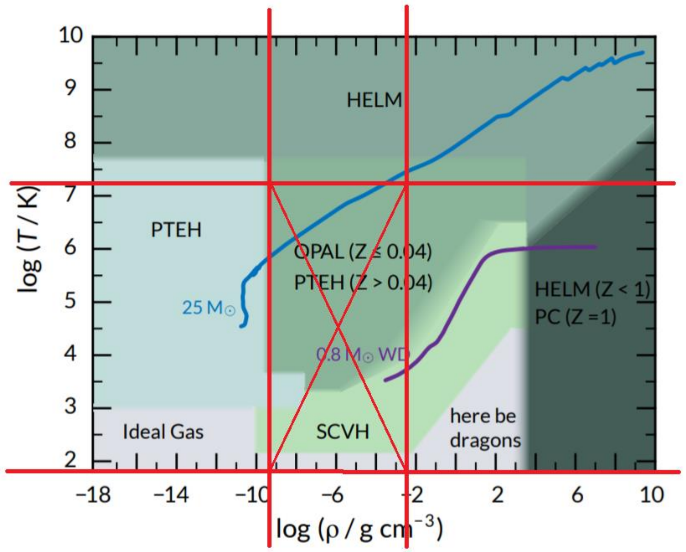
- Limitation…
  - Consider elements up to neon (anything heavier then neon is neon)
  - Relative abundance of heavier elements (ignore H and He)

Element	Relative mass Fraction	Relative number fraction
C	0.1906614	0.2471362
N	0.0558489	0.0620778
O	0.5429784	0.5283680
Ne	0.2105114	0.1624178

  - above $T \sim 10^9$ K: pair production becomes an issue
  - Below $T \sim 5000$ K: numerical difficulty
  - Above $\rho \sim 10^5$ g cm^{-3}: electron are relativistic.



SCVH



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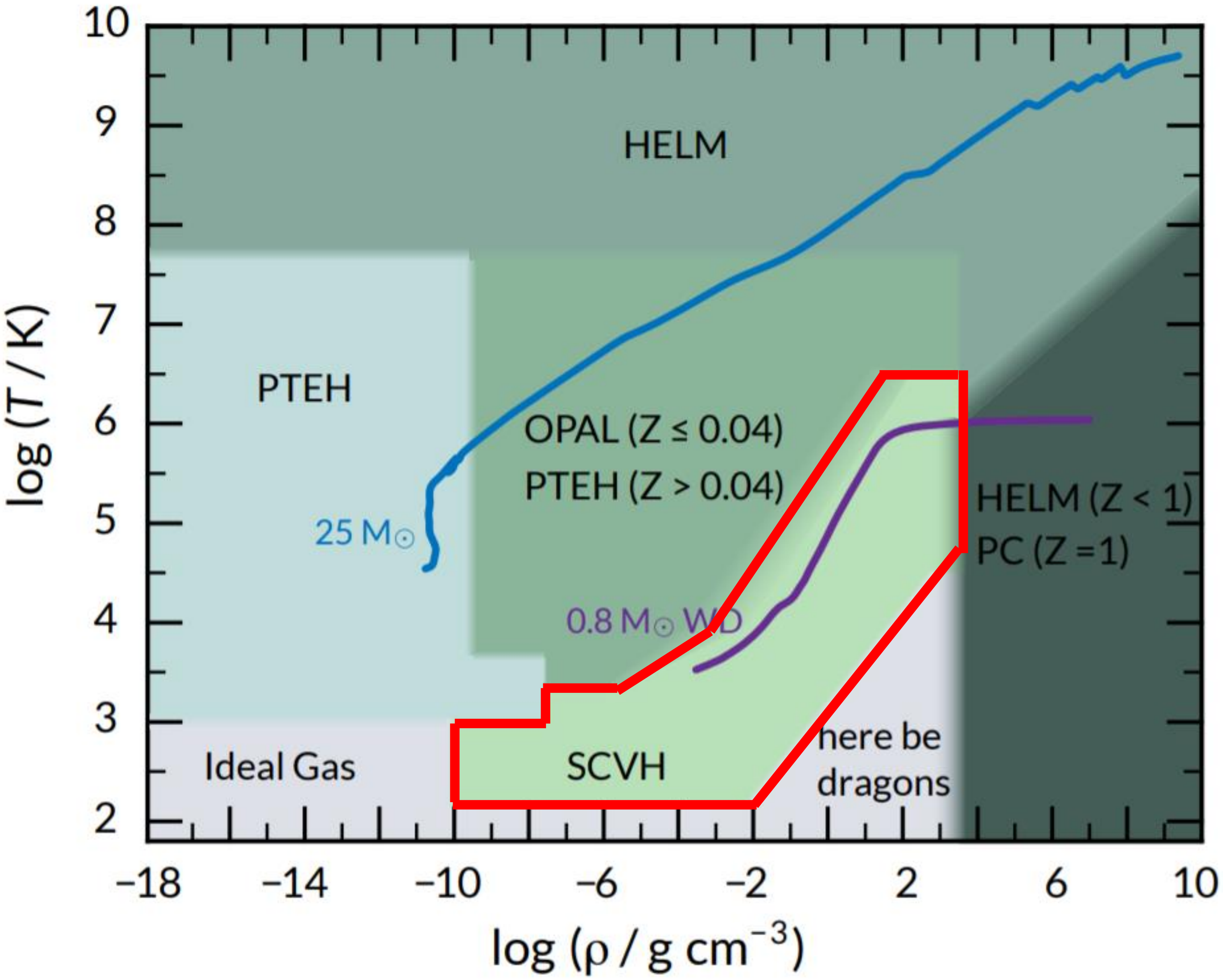

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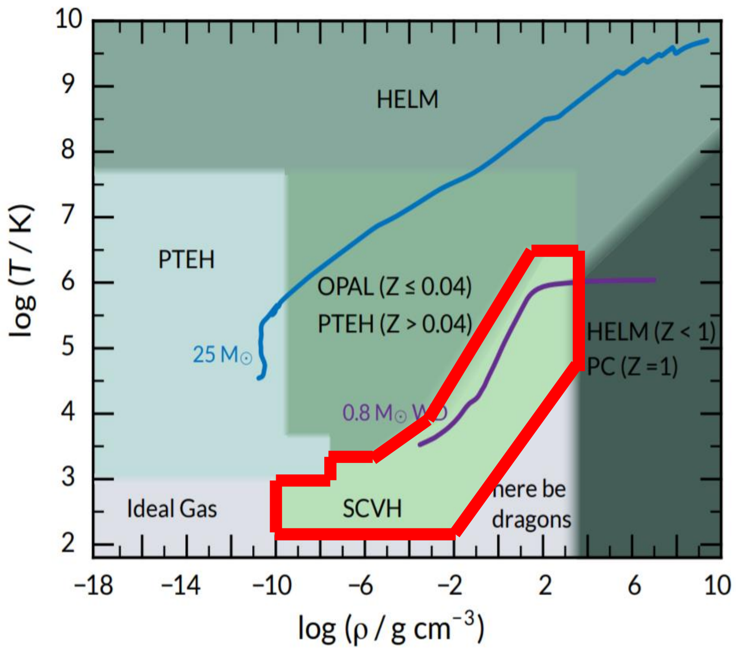
SCVH EOS

- Considers …
  - "chemical picture"
  - Uses " (Helmholtz) free energy minimization method" $F = U - TS$
  - Obtained a EOS for pure hydrogen; a EOS for pure helium
  - Interpolate to get values in between

- Excludes all heavier elements (Z=0)



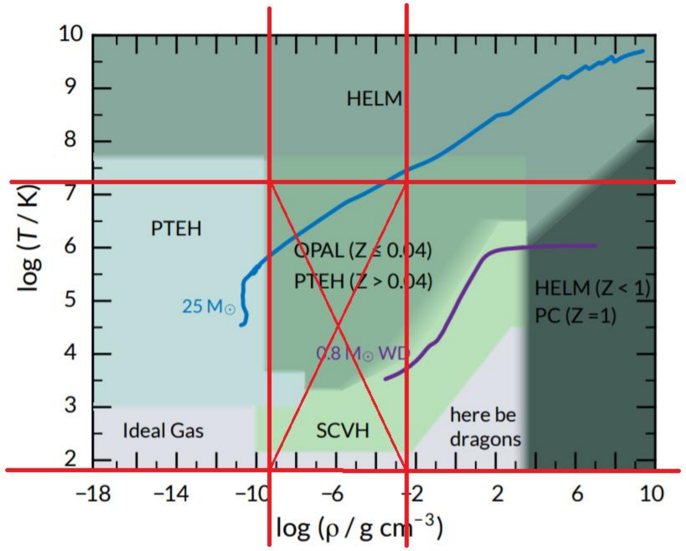
SCVH EOS

- Hydrogen
  - "plasma phase transition" (PPT): Pressure ionization occurs discontinuously through first-order phase transition (at $\log T_c \sim 4.185$)
  - Considers H, H^+, H_2, e
  - Accounts for weak diffraction in the interaction of heavy particles

- Helium
  - Also considers Helium PPT
  - Considers He, He^{2+}, He^+, e

- In between
  - Interpolation and approximation

PTEH



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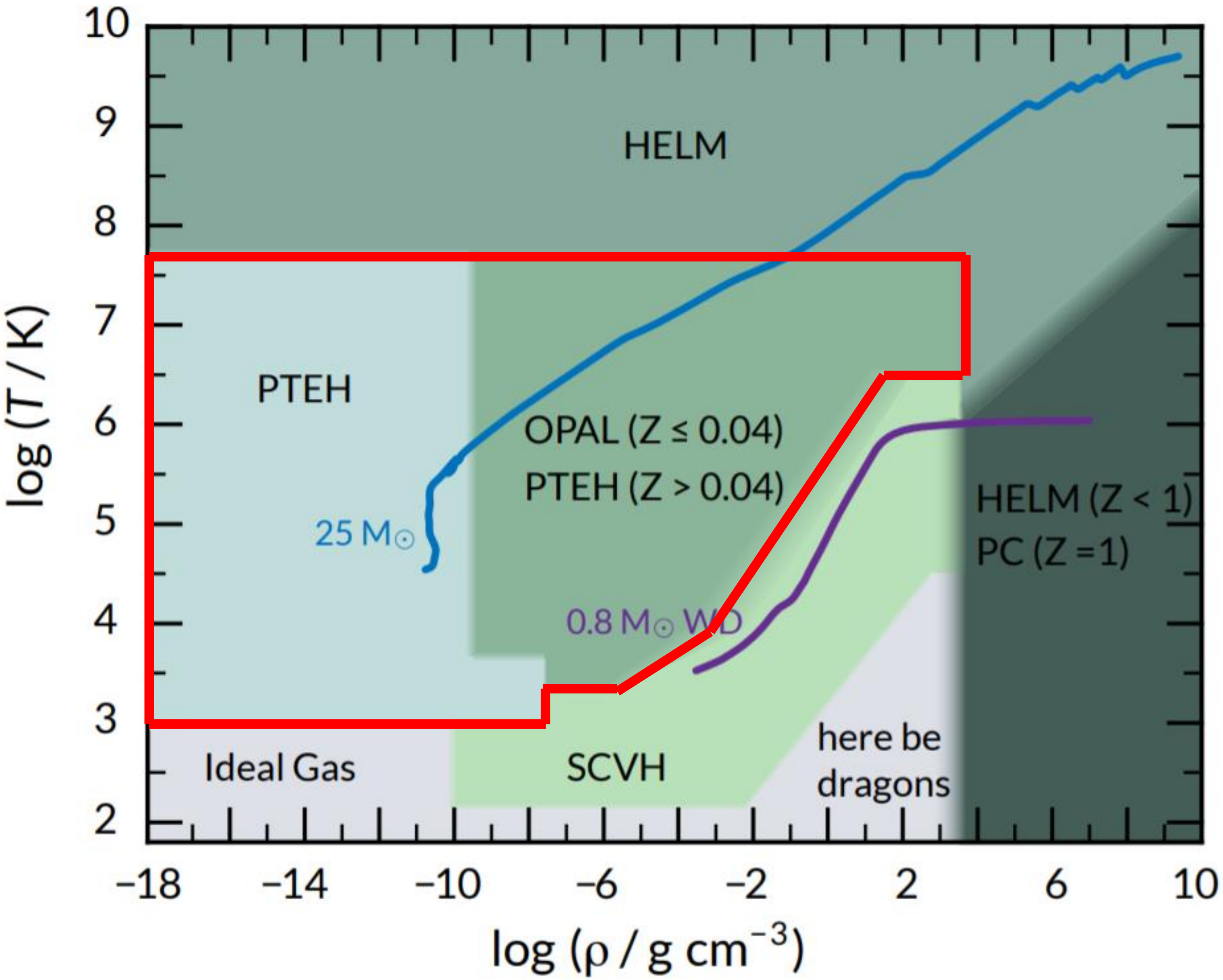

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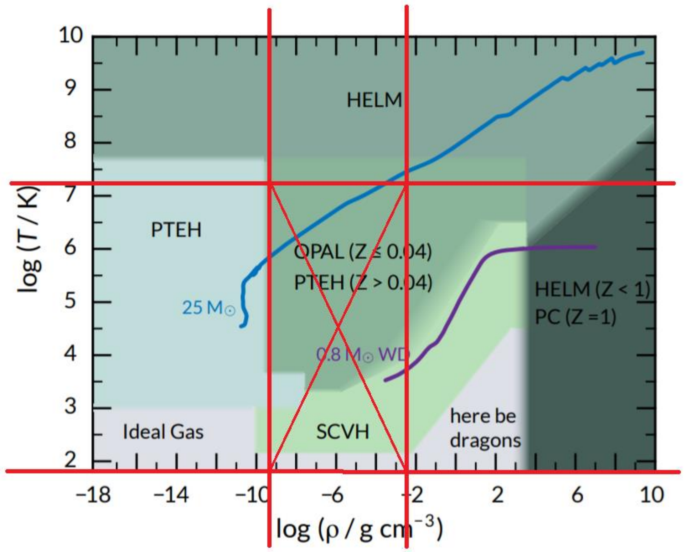
PTEH EOS

- Based on Helmholtz free energy minimization
- Elements included are H, H^{+} ,H_2 , He^{2+}, He^{+}, He, e; as well as 7 heavier elements C, N, O, Ne, Mg, Si and Fe, which are assumed to be fully ionized, at all temperature and density.
- Heavy elements effects EOS insignificantly; but influences opacity greatly

HELM



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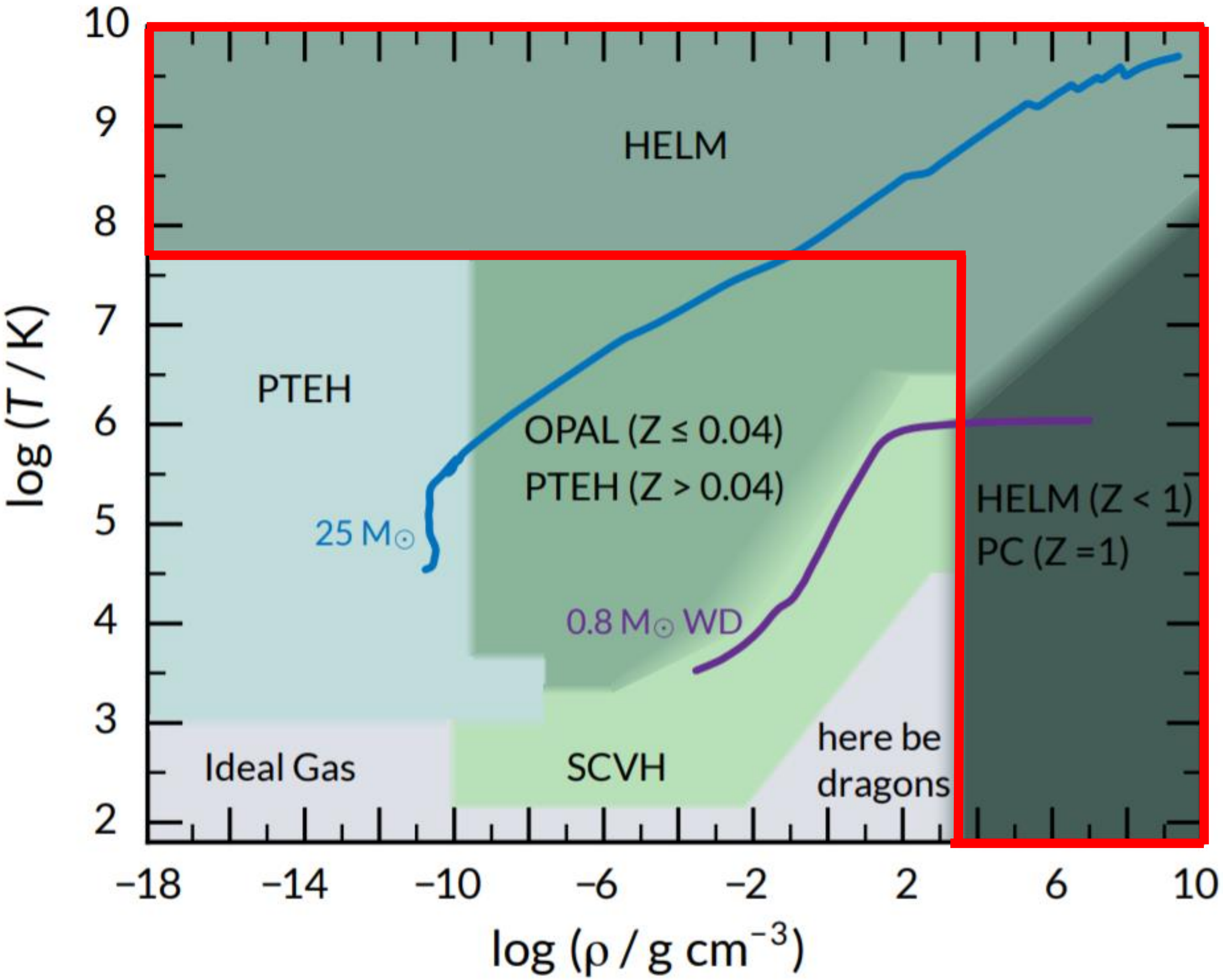

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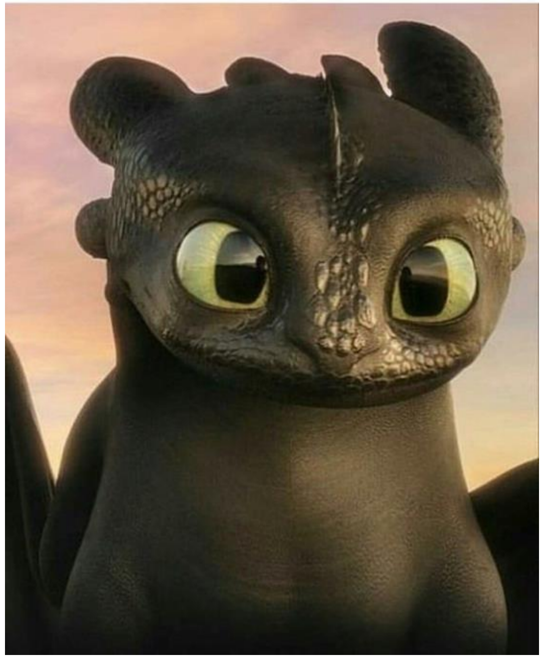
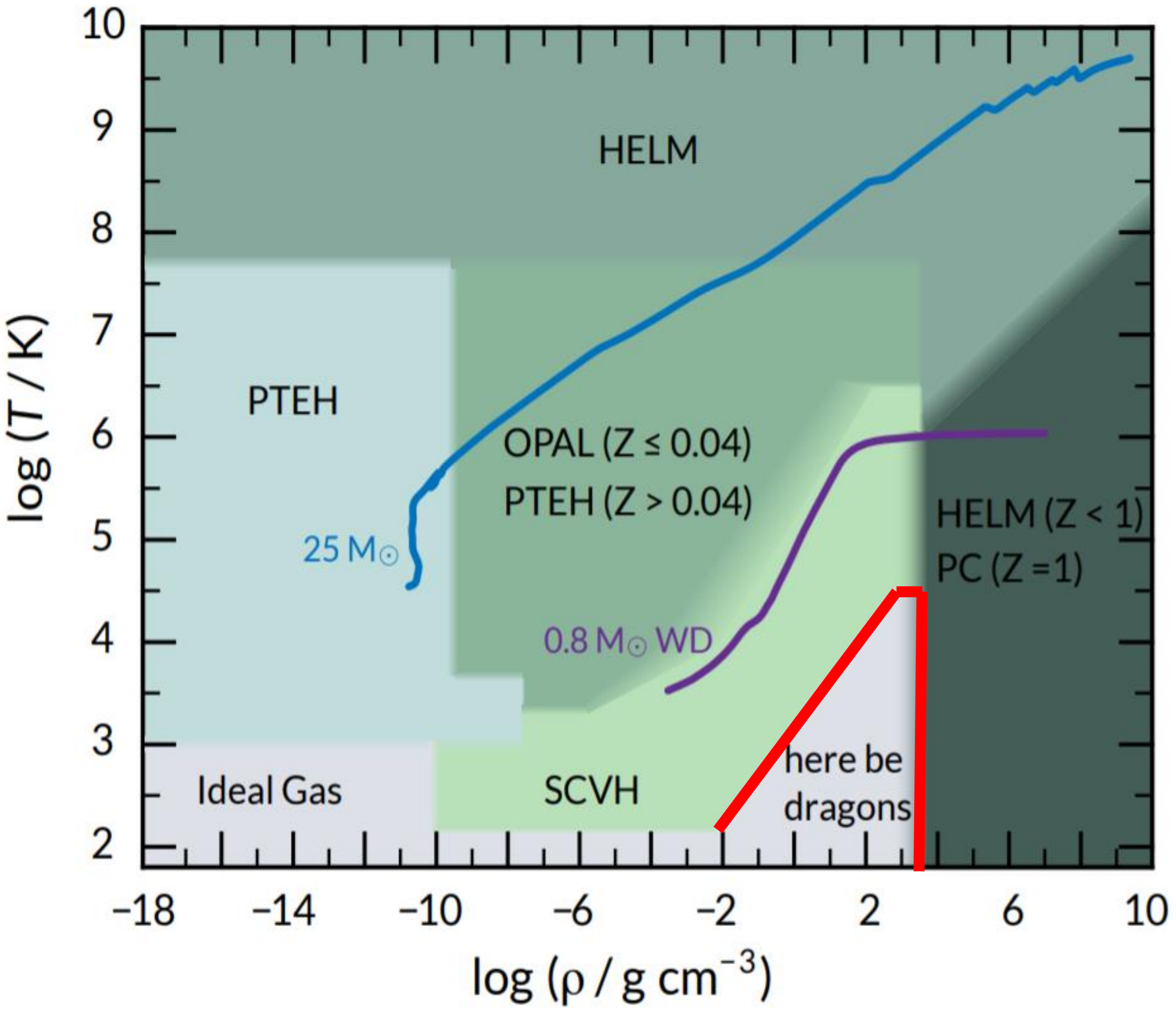
HELM EOS

- Assume fully ionized gas (at very high temperature or density)
- Deals with electron-positron physics
- Based on Helmholtz free energy

Dragons





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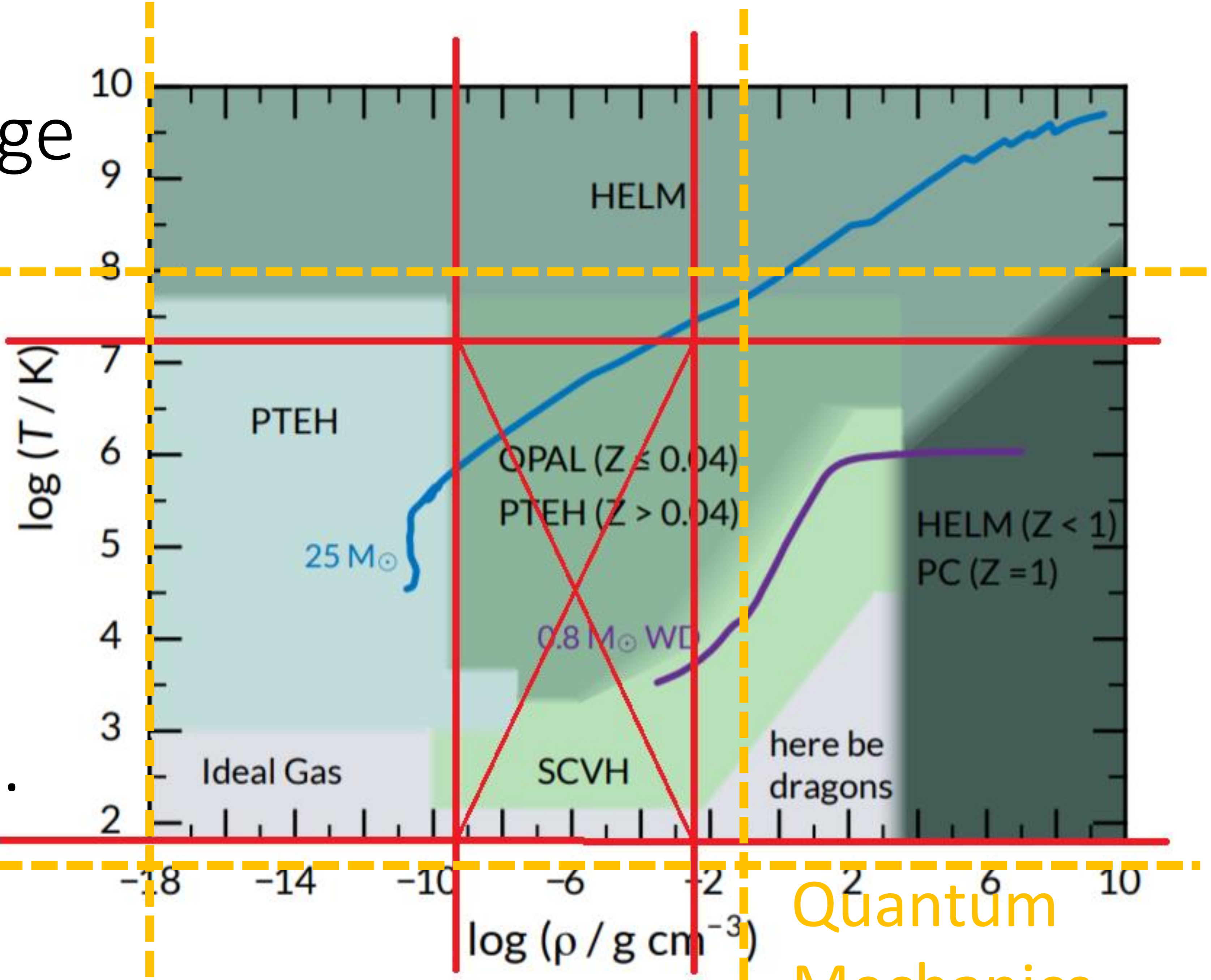
Proposed range

Pair production



Physical & monotone

One more thing …

Metallicity

Quantum Mechanics

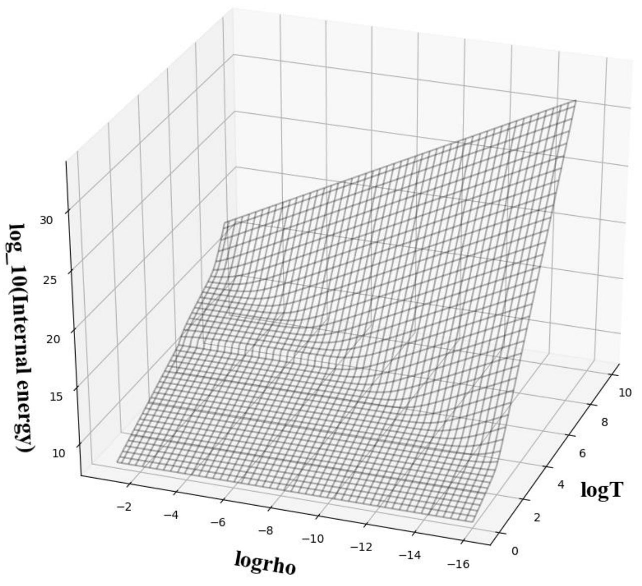
One last thing … Metallicity

- Slight variation in Metallicity is insignificant for EOS, but impacts greatly for opacity
- Solar metallicity
  - $X \sim 0.74$
  - $Y \sim 0.25$
  - $Z \sim 0.0134$
- High-metallicity star: $Z \sim 0.03$, theoretically people considers up to $Z \sim 0.05$
- Helium abundance goes up to $Y \sim 0.42 \pm 0.1$ for very old star cluster. Typical value close to that of the sun

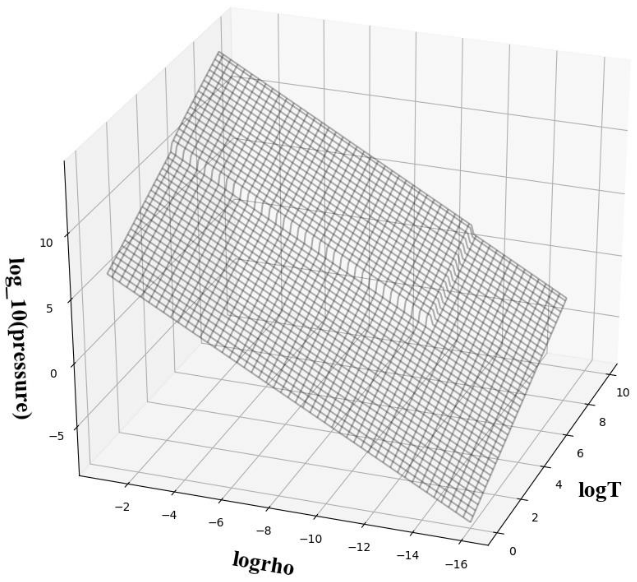
Ref: Big orange book (Carroll & Ostlie), Pg 474 sec. 13.3
Ref: AAS 106, 275-302 (1994)
http://articles.adsabs.harvard.edu/pdf/1994A%26AS..106..275B
Ref: (Y abundance)
https://arxiv.org/ftp/arxiv/papers/0811/0811.2980.pdf

$$-18 \leq \log \rho \leq -1 \qquad 0 \leq \log T \leq 8$$
$$(Z = 0.02)$$

$E(\rho, T)$



$P(\rho, T)$

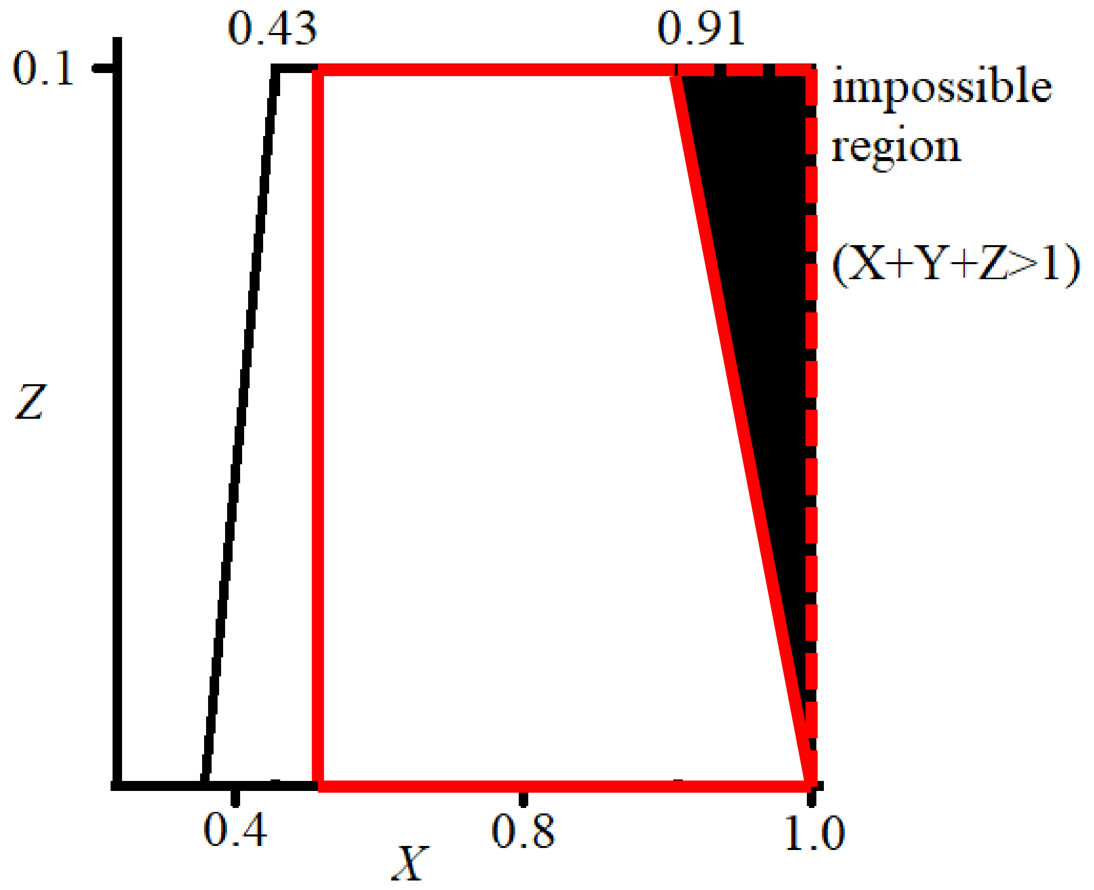


$P(\rho, T)$ and $E(\rho, T)$ are both monotone

- Monotonicity implies that in the range we choose, if we have two parameters out of $\{\rho, T, P, E\}$, then the other two are uniquely defined.
- In other words, we only need two tables to create all others.

$$-18 \leq \log \rho \leq -1 \qquad 0 \leq \log T \leq 8$$
$$\text{EOS is monotone } \forall X \geq 0.5, 0 \leq Z \leq 0.1$$

- Proposed metallicity range
  - $0 \leq Z \leq 0.1$
  - $0.5 \leq X \leq 1$
  - This leads to $0 \leq Y \leq 0.5$
  - MESA is able to produce the tables in the unphysical region… (without warning)



Currently available EOS tables

- $P(\rho, T)$ (MESA)
- $E(\rho, T)$ (MESA)
- $T(\rho, P)$
- $T(\rho, E)$

- $C_s(\rho, T)$ (MESA)
- $C_V(\rho, T)$ (MESA)

- Can be calculated indirectly…
  - $P(\rho, E) = P\big(\rho, T(\rho, E)\big)$
  - $E(\rho, P) = E\big(\rho, T(\rho, P)\big)$

- Metalicity
  - $X = 0.5, 0.6, 0.7, 0.8, 0.9, 1.0$
  - $Z = 0.0, 0.02, 0.04, 0.06, 0.08, 0.10$

Next step

- Putting EOS into AstroBEAR
  - For tabulated $z(x, y)$, at any (x_0, y_0), we can get the corresponding z_0
- Test EOS

Additional info

- Metallicity: for an arbitrary (X, Z), using sampled values to approximate thermodynamical quantities differs by at most 0.05 from data directly obtained from MESA. (except around $X = 1$, the difference goes up to 0.2 due to numerical difficulties).

- Metalicity
  - $X = 0.5, 0.6, 0.7, 0.8, 0.9, 1.0$
  - $Z = 0.0, 0.02, 0.04, 0.06, 0.08, 0.10$

Inversion algorithm

- Let $f = z(x, y)$ be a monotone function where z is defined on a rectangular parameter space.
- Since the data is discrete, consider $\{z_{x1}(y), z_{x1}(y), z_{x1}(y) \ldots\}$ where z_{xi} is the slice at $x = x_i$. Reducing the variables to 1D
- Now, at the new parameter space (x, z), define an "error function" on each "sample point" z_0: $\mathrm{ERR}(y) = |z(y) - z_0|$ where y is the corresponding y at z_0. Minimize $\mathrm{ERR}(y)$ to get the best fit using Nelder-Mead algorithm.
- Sometimes in the python function the guess value will exceed the limitations of the table. So a "pseudo-function" is implemented to extend $\mathrm{ERR}(y)$ to greater region (assume linear at the end)
- Do this for all $z_0 \in$ new parameter space, and we get the inverted table.

Inversion algorithm

- Let $f = z(x, y)$ be a monotone function where z is defined on a rectangular parameter space.
- The inversion outputs $g = y(x, z)$. Some values on the rectangular parameter space (x, z) has no corresponding value. We use nan to take the place
- If we invert g function again to obtain $h = z_2(x, y)$. Then compare $f - h$, the difference is less then 0.05 at all times (numerical difference, not percentage). It appears that the inverting algorithm only have difficulties where on the original function the first derivative is not continuous (otherwise the difference is practically 0).