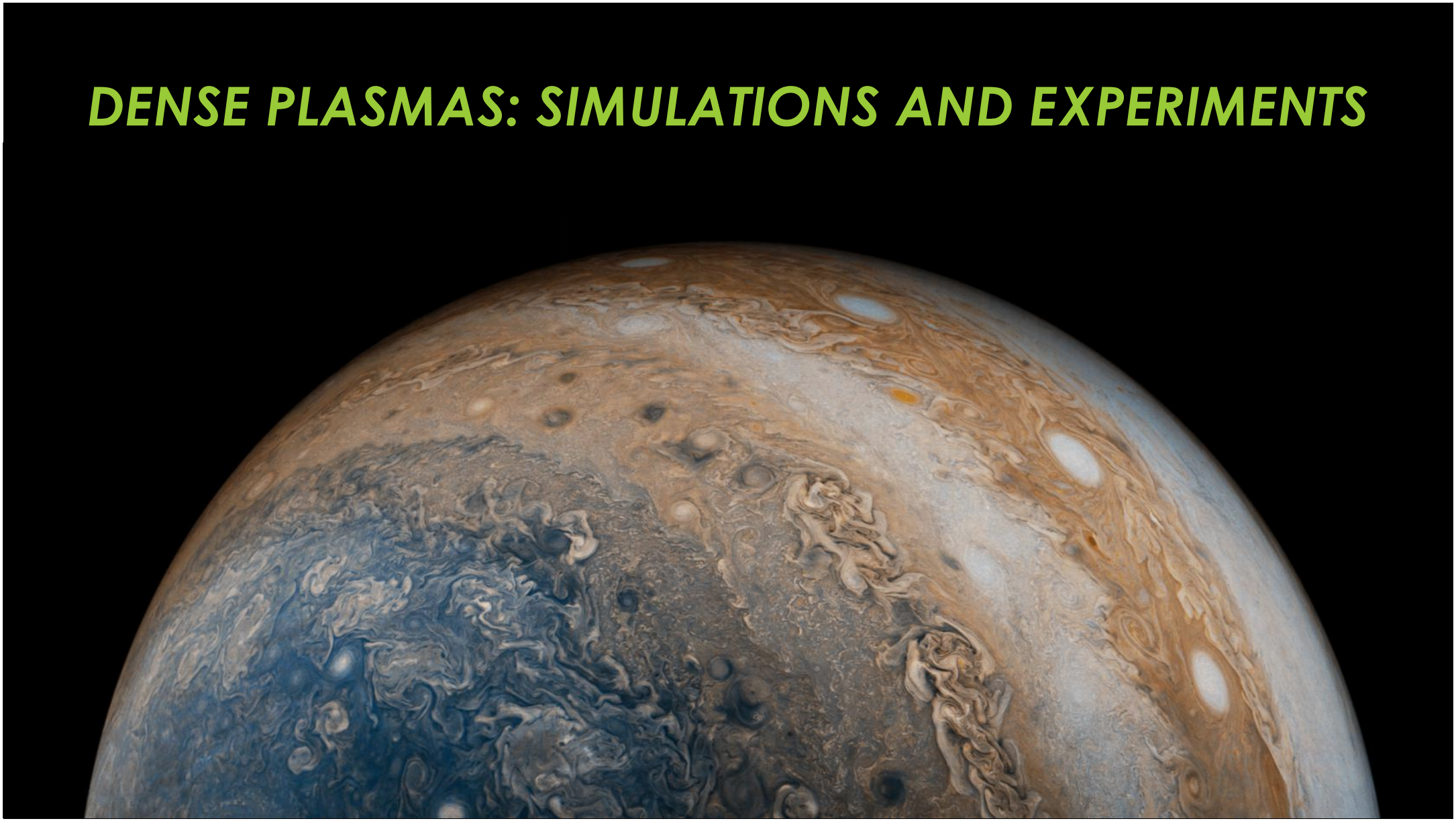
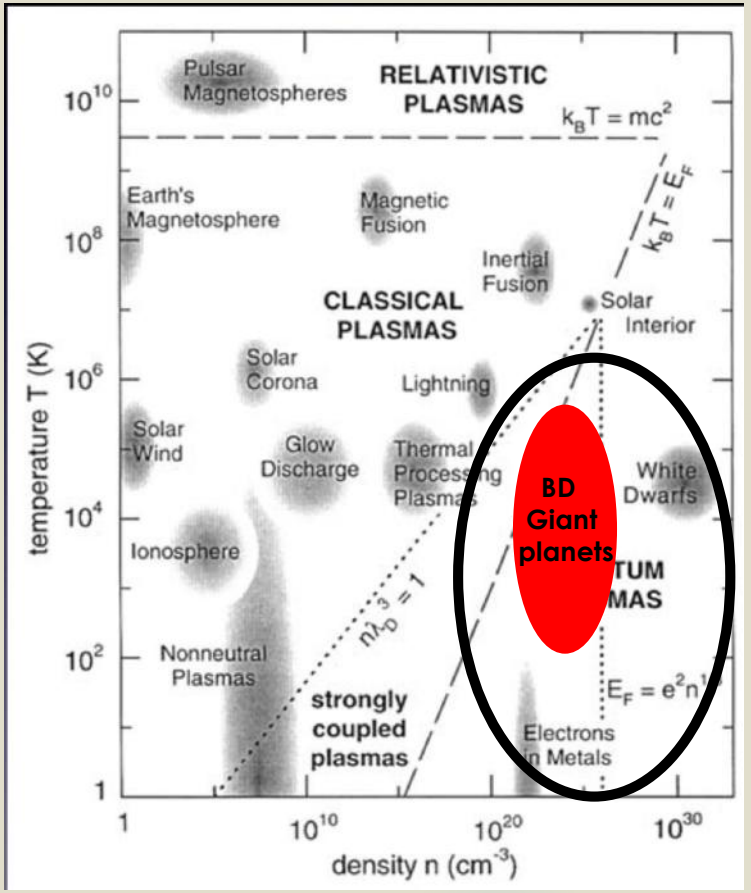
DENSE PLASMAS: SIMULATIONS AND EXPERIMENTS



Astroplasma

Looking for someone on
the white dwarf/neutron star thematics



Overview

I. *Simulations*

II. *Experiments*

III. *Comparison with EOS*

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. Dirac, 1929

I. Simulations

Even for H or He: non zero temperature quantum effect impossible to solve

Three main numerical method developped in the XXth century:

Path Integral Monte Carlo **Quantum Monte Carlo** **Density Functional Theory**

I. Simulations

Path Integral Monte Carlo (or Path Integral Molecular Dynamics) evaluate ion and electron motion (at the expense of numerical cost)

QMC and DFT solve the electronic problem but **must be coupled to an evolution for the ions** (most of the time, classical molecular dynamics)

I will not detail QMC, based on trial wave functions to optimize the energy. See McMahon et al. 2012

I. Simulations

PIMC

Objective: calculate the partition function

$$Z = \mathrm{Tr}(e^{-\beta H})$$

With $\beta = \frac{1}{k_B T}$ and H the Hamiltonian, $e^{-\beta H}$ is the density matrix

I. Simulations

PIMC

Why Z ?

In the canonical ensemble: $F = -k_B T \ln Z$

$$P = -\left.\frac{\partial F}{\partial V}\right|_{T,N}, S = -\left.\frac{\partial F}{\partial T}\right|_{V,N}$$

I. Simulations

PIMC

Hypotheses: $H = T + V$, kinetic + potential

$$T = \sum_{i=1}^{N} -\frac{1}{2m_i}\hat{\nabla}^2 \ , \qquad V = \sum\nolimits_{i<j} \frac{z_i z_j}{|\vec{r_i} - \vec{r_j}|}$$

Potential operator only depend on position

I. Simulations

PIMC

Rewriting: $Z = \mathrm{Tr}(e^{-\beta H})$, $\varrho = e^{-\beta H}$ with the Hamiltonian eigenfunctions:

$$\varrho(R, R'; \beta) = < R \left| e^{-\beta H} \right| R' > = \sum_i \phi_i{}^*(R)\phi_i(R')e^{-\beta E_i}$$

$$Z = \int \varrho(R, R; \beta) dR$$

R: positions of the ensemble of particles

I. Simulations

PIMC

Basics of PIMC :

$$e^{-(\beta_1+\beta_2)H} = e^{-\beta_1 H} e^{-\beta_2 H}$$

Denoting $\tau = \frac{\beta}{M}$, $e^{-\beta H} = (e^{-\tau H})^M$

$$\varrho(R_0, R_M; \beta) = \int \varrho(R_0, R_1; \tau) \dots \varrho(R_{M-1}, R_M; \tau) dR_1 \dots dR_{M-1}$$

$$Z = \varrho(R_0, R_0; \beta)$$

Z does not depend on the path (R0-> R0). MCMC sampling of the possible paths to evaluate the integral. Why is that better than just calculating integral?

I. Simulations

PIMC

Simplified expression for the density matrix at high temperature

$$e^{-\tau T}e^{-\tau V} = e^{-\tau(T+V)+\frac{\tau^2}{2}[T,V]} \rightarrow e^{-\tau(T+V)}$$

And there is no build up second order error (Trotter 1959):

$$e^{-\beta(\boldsymbol{T}+\boldsymbol{V})} = \lim_{M\to\infty}[e^{-\tau T}e^{-\tau V}]^M$$

At high temperature, decouple kinetic and potential energies

I. Simulations

PIMC

General form of PIMC (from Ceperley 1995):

$$\varrho(R_0, R_M; \beta) = \int \exp\left(-\sum_{m=1}^{M} S_m\right) dR_1 \dots dR_{M-1}$$

S is the action.

With Trotter, we impose the *primitive approximation* (commutation of kinetic and potential action):

$$\varrho(R_0, R_M; \beta) = \int \exp\left(-\sum_{m=1}^{M} \frac{(R_{m-1} - R_m)^2}{4\lambda\tau} + \tau V(R_m)\right) (4\pi\lambda\tau)^{-3NM/2} \, dR_1 \dots dR_{M-1}$$

I. Simulations

PIMC

$$\varrho(R_0, R_M; \beta) = \int \exp\left(-\sum_{m=1}^{M} \frac{(R_{m-1} - R_m)^2}{4\lambda\tau} + \tau V(R_m)\right)(4\pi\lambda\tau)^{-3NM/2}\, dR_1 \dots dR_{M-1}$$

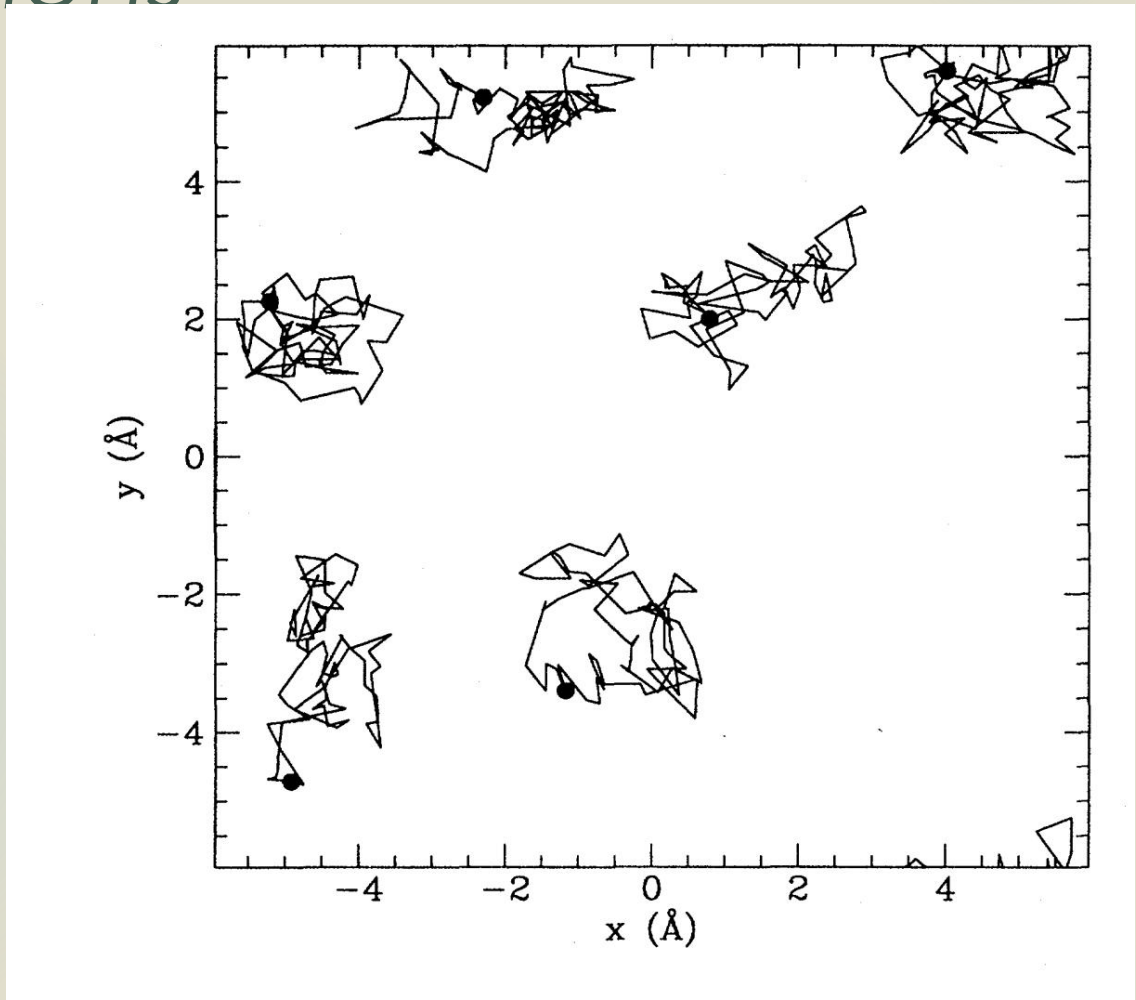
Classical analogy:

Kinetic action is a string potential between the same atom at different time slice => polymers.

Potential action is a repulsion potential between polymer at the same time

$Z = \varrho(R_0, R_0; \beta)$: ring polymers !

I. Simulations

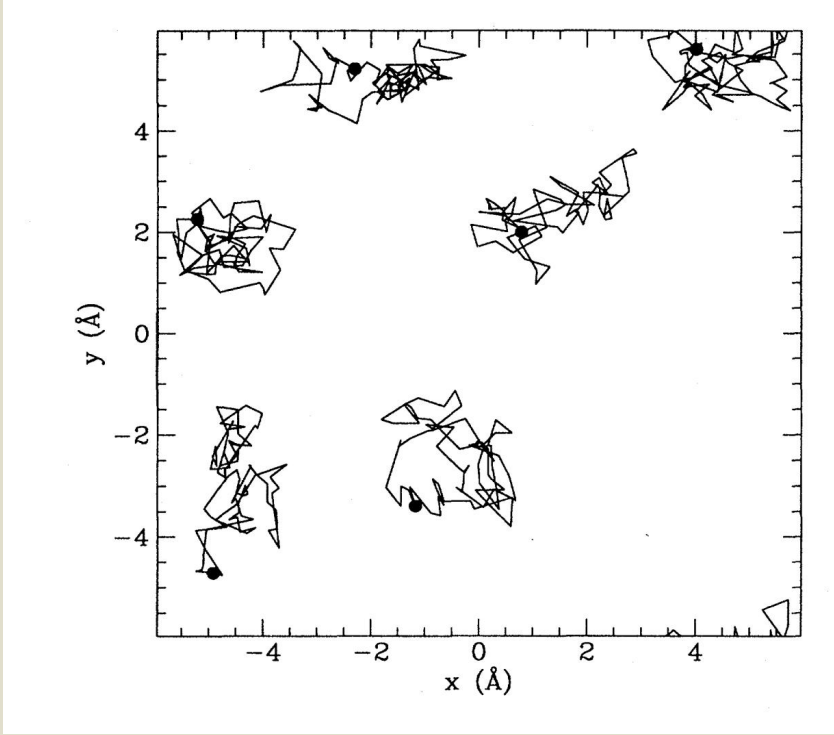


I. Simulations

PIMC

The partition function is the same in quantum PI and classical analogy: PIMC samples the possible paths, and consider it as a classical thermodynamical system.

Real difficulty: good strategy for MCMC acceptable sampling of the path.



I. Simulations

PIMC

Uncer certain approximations (free energy Born-Oppenheimer approximation, Feynman and Hibbs 1965, Cao and Berne 1993):

$$Z = \oint \mathfrak{D}\vec{R} exp[-\int_0^\beta dt(T\left(\vec{R}(t)\right) + F_{el}(\vec{R}(t))]$$

We recover the ion-electron separation: electron free energy can be calculated with DFT of QMD, and ion movements with PIMC

I. Simulations

DFT

Hohenberg-Kohn theorems:

1) There is a one to one correspondance between the external potential (from the nuclei) and the ground-state electronic density.

2) There exists a universal energy functional of the density, defined for any potential, such that the global minima of this functional represents the ground-state energy of the system.

I. Simulations

DFT

Obvious problem: functional not known. Most used simplification: Kohn and Sham 1965:

$$E_{KS}(n) = -\frac{1}{2}\sum_{i=1}^{N}\left|\vec{\nabla}\varphi_i(\vec{r})\right|^2 + \int V_{ext}(\vec{r})n(\vec{r})d^3\vec{r} + \frac{1}{2}\int \frac{n(\vec{r})n(\vec{r'})}{\left|\vec{r}-\vec{r'}\right|}d^3\vec{r}d^3\vec{r'} + E_{NN} + E_{xc}(n)$$

E_{xc} accounts for exchange and correlation: unknown

I. Simulations

DFT

Some ways to corect for finite temperature (Mermin 1965).

What is E_{XC} ?

Answer: fitted with experiments and situation

For dense hydrogen, most used is the Perdew-Burke-Ernzerhof (Perdew, Burke and Ernzerhof 1996).

I. Simulations

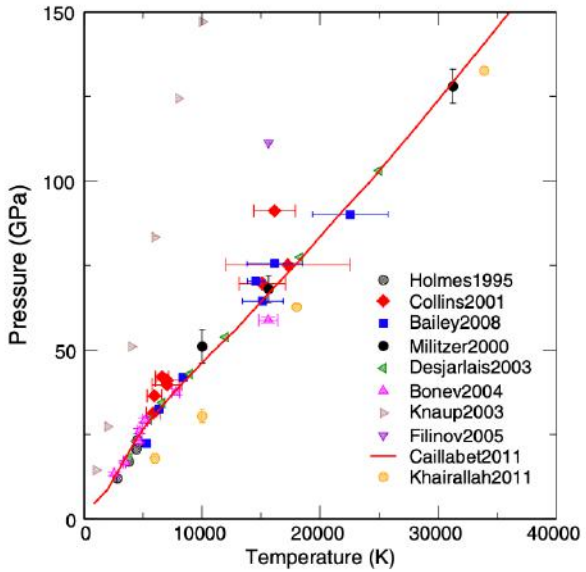


FIG. 12 (color online). Pressure vs temperature along the Hugoniot. Comparison among experimental data and various theoretical predictions. Experiments: gas-gun [shaded circles (Holmes, Ross, and Nellis, 1995)], Nova laser [diamonds (Collins, Celliers *et al.*, 2001)], Z pinch [squares (Bailey *et al.*, 2008)]. Theory: RPIMC [closed circles (Militzer and Ceperley, 2000), light shaded circles (Khairallah, Shumway, and Draeger, 2011)], BOMD [left triangle (Desjarlais, 2003), up triangle (Bonev, Militzer, and Galli, 2004), line (Caillabet, Mazevet, and Loubeyre, 2011)], direct PIMC [down triangle (Filinov *et al.*, 2005)] and WPMD [right triangle (Knaup *et al.*, 2003)].

Some results

Precise knowledge of Jupiter requires errors < 1%(Stevenson 2010)

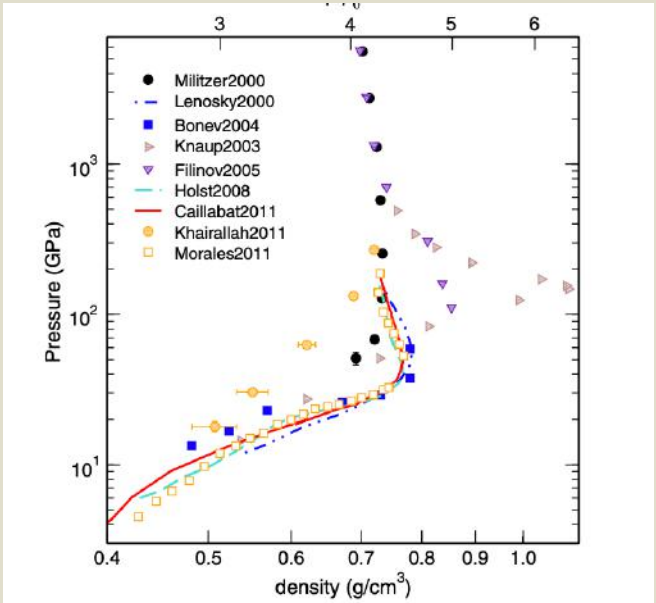
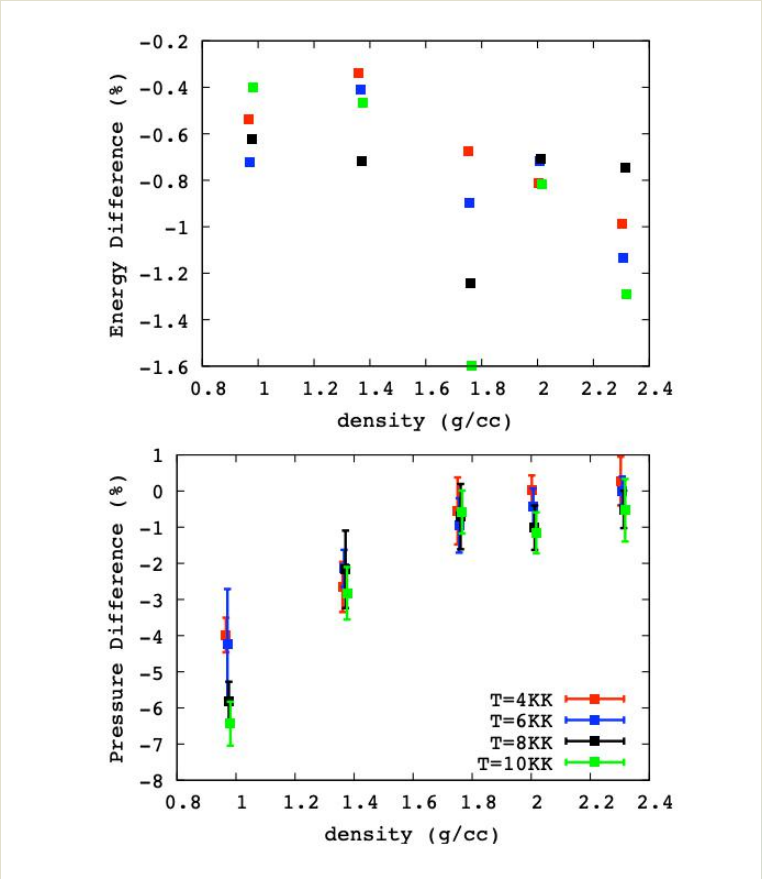


FIG. 13 (color online). Comparison among various theoretical methods of computations of the principal Hugoniot for deuterium. RPIMC (dark closed circles) (Militzer and Ceperley, 2000), (light closed circles) (Khairallah, Shumway, and Draeger, 2011) and direct PIMC (down triangles) (Filinov *et al.*, 2005). FPMD ground-state electrons (double dot-dashed line) (Lenosky *et al.*, 2000), (closed squares) (Bonev, Militzer, and Galli, 2004b) and thermal electrons (dashed line) (Holst, Redmer, and Desjarlais, 2008), (continuous line) (Desjarlais, 2003; Caillabet, Mazevet, and Loubeyre, 2011) and (open squares) (Morales *et al.*, 2012). WPMD (right triangle) (Knaup *et al.*, 2003).

I. Simulations

Some results

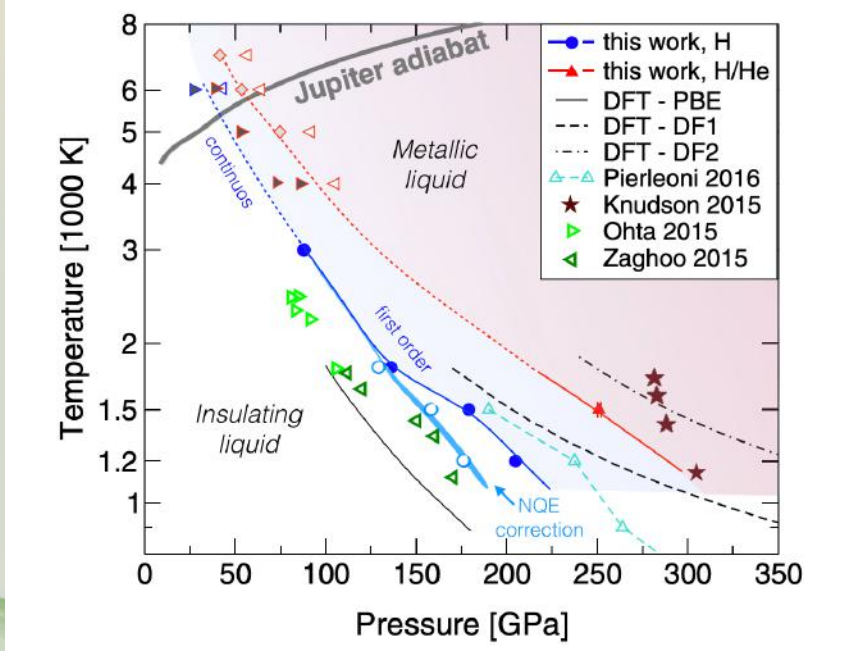
Morales et al. 2009:
EOS based on QMD
Difference with DFT

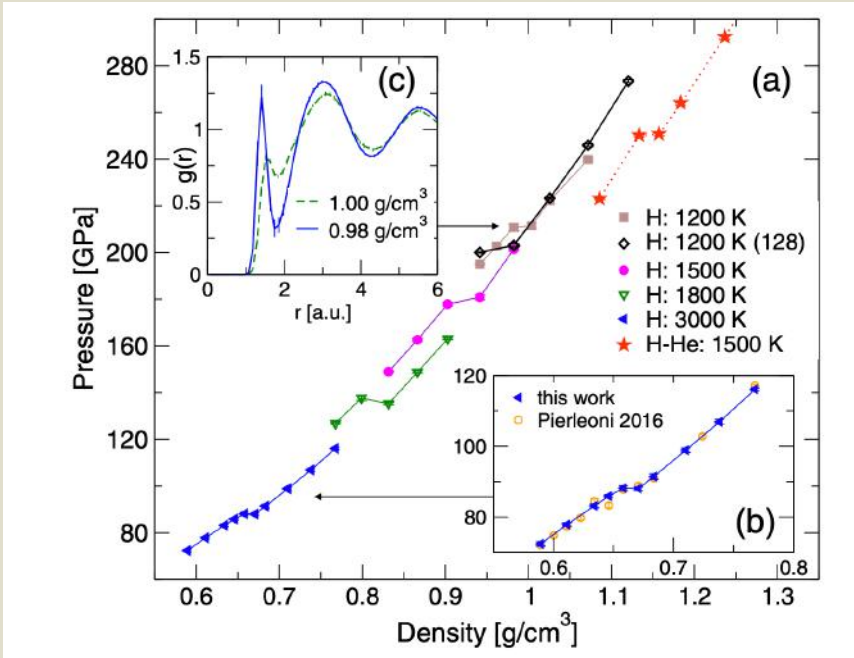


I. Simulations

Some results

Numerical first order
PPT ?



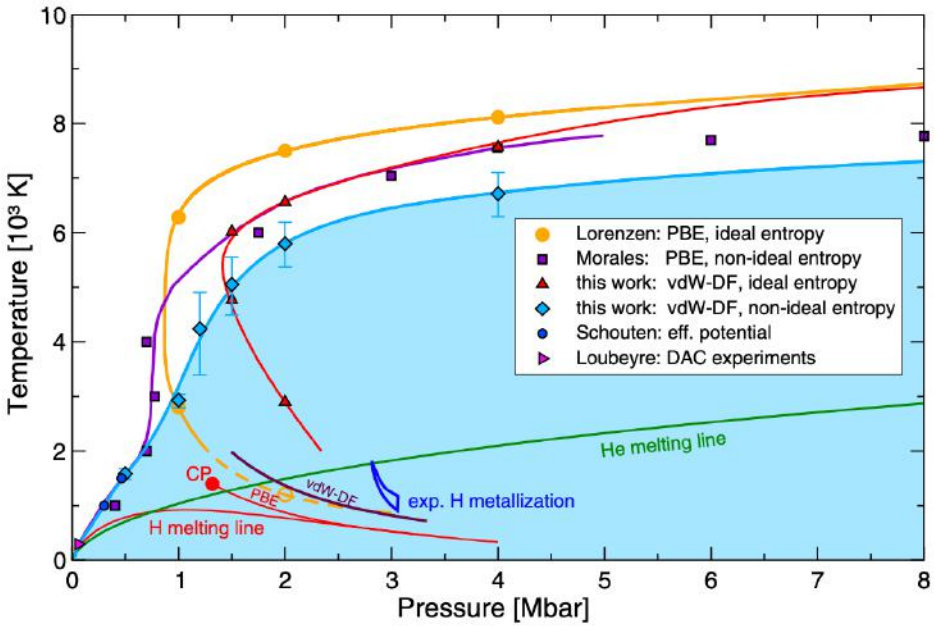


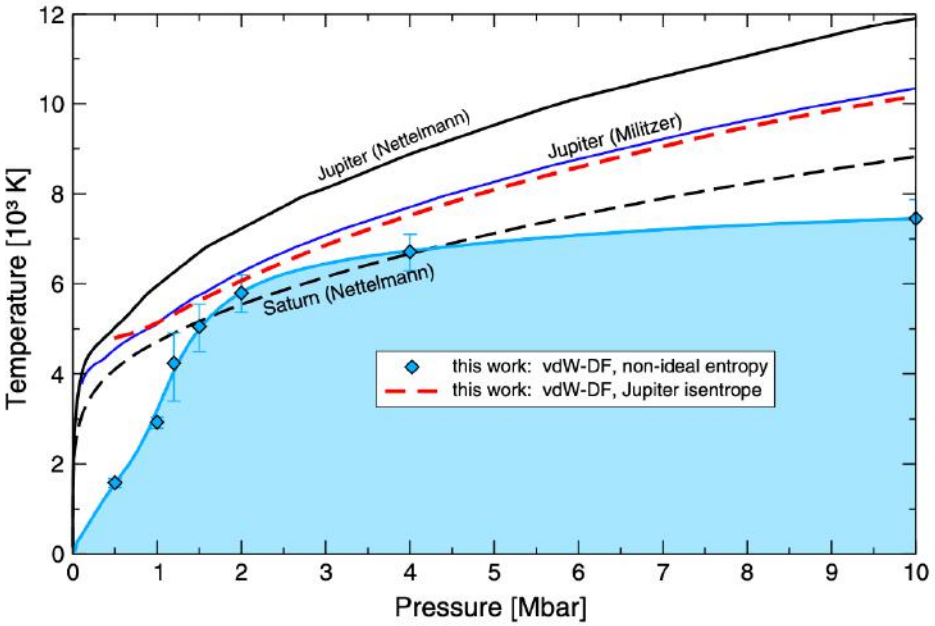
Mazzola et al. 2018

I. Simulations

Some results

H-He immiscibility:



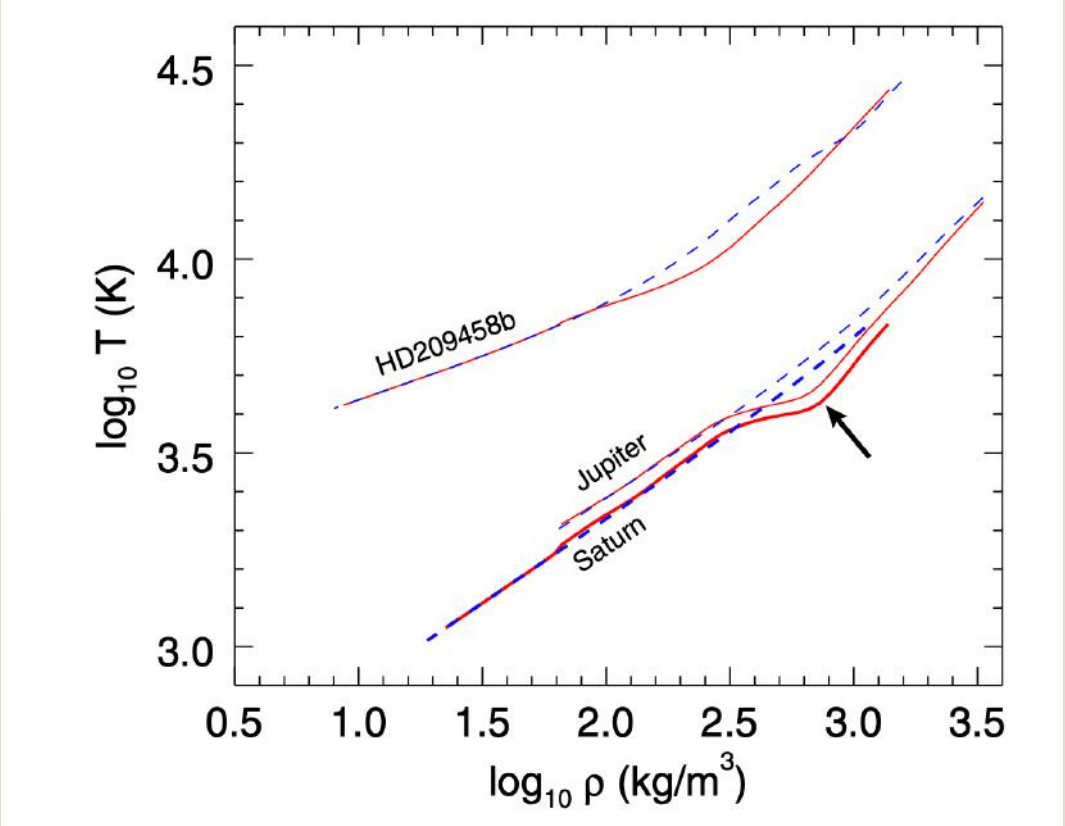


I. Simulations

Some results

Militzer & Hubbard 2013:
Non ideal H-He mixing

Finite size effects ?
220 H – 18 He



II. Experiments

Goal: reliable estimates of thermodynamic quantities of compressed H / He

Metallic hydrogen: the « holy grail » of high pressure research

1) Verification of quantum mechanics
2) Verify numerical simulations for other material
3) Most abundant element (+ giant planets and stars)

II. Experiments

Two main methods: static / dynamic compression

Difficulty: diffusivitiy of hydrogen, breaks the setup and explodes …

Not my field of expertise ..

Extended review by Nellis 2006. See also Mcmahon et al. 2012,

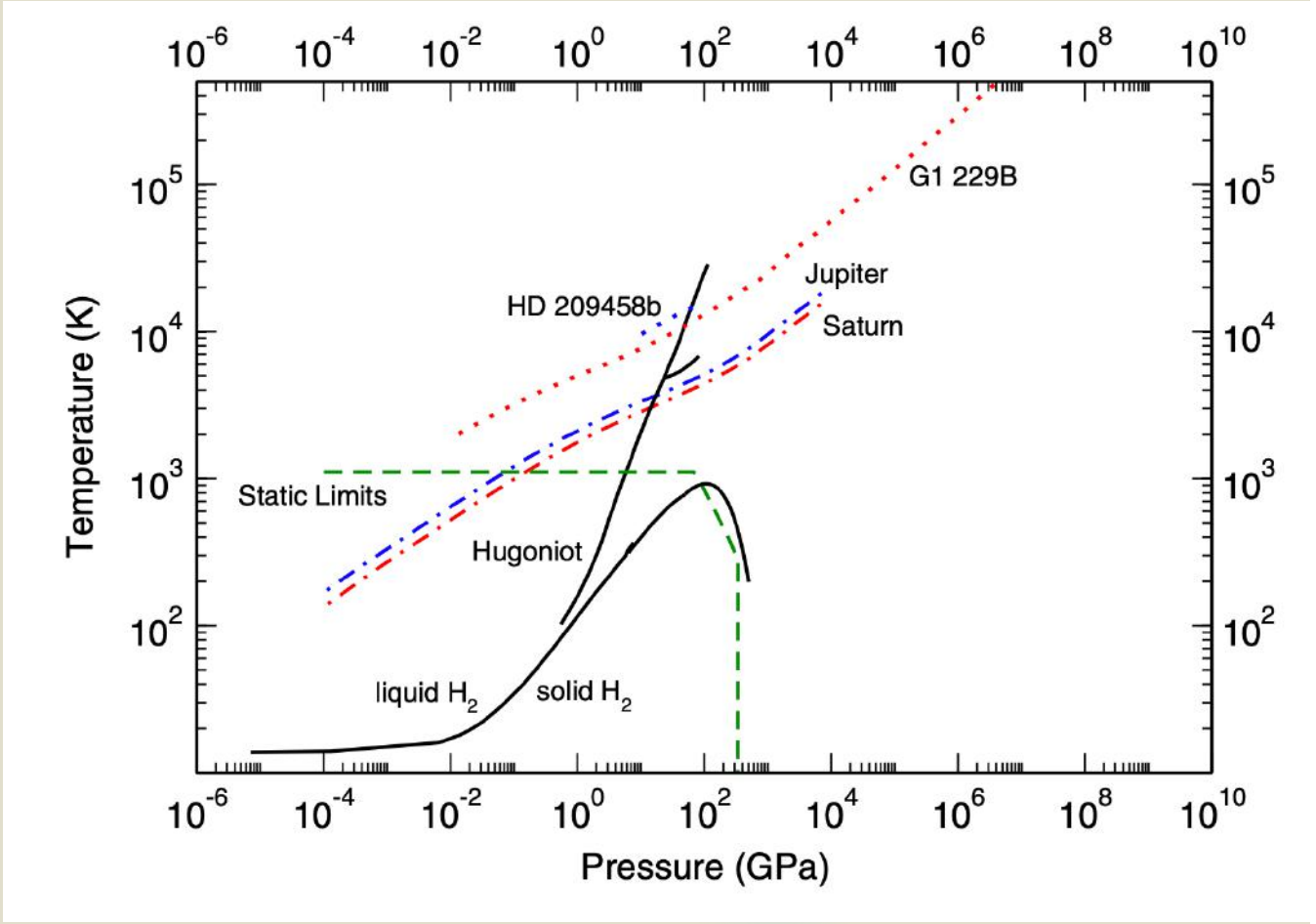
II. Experiments

Static compression: diamond anvil cell.

Dynamic compression: laser shock, gun gas

2012

Both static and dynamic limits pushed further



II. Experiments

Difficulty with experiments: metallic H becomes very reflective. Complicates measurements

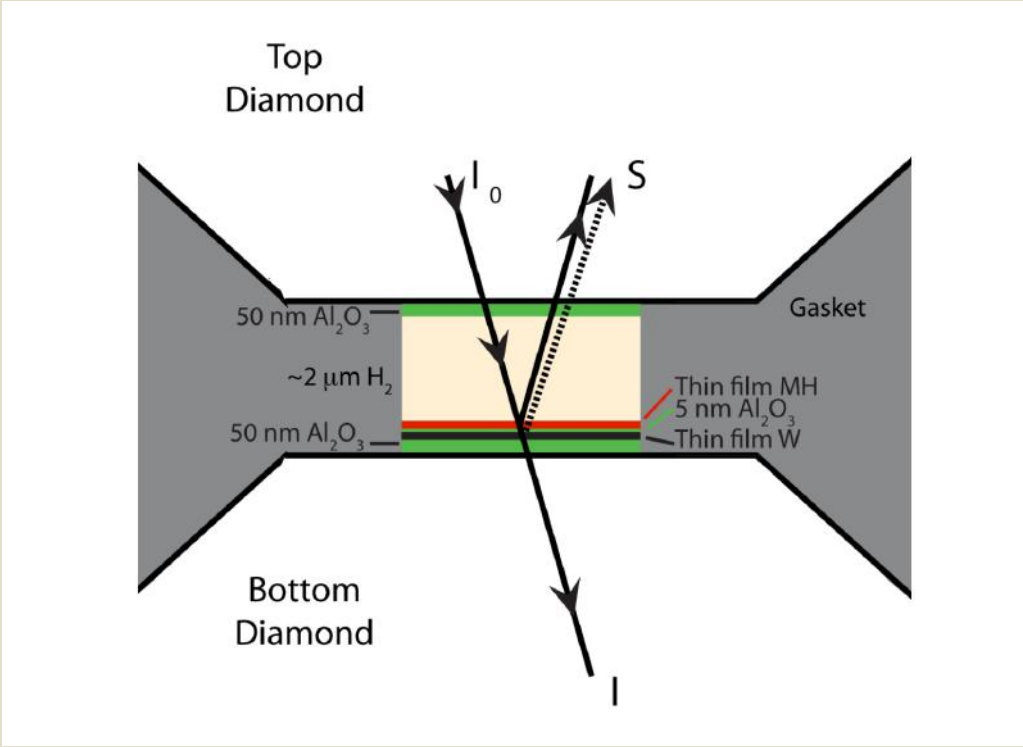
Problem: lots of claims, lots of debate.

Phase diagram unknown: we don't know when metallisation occurs

II. Experiments

Reflectance measure from DAC

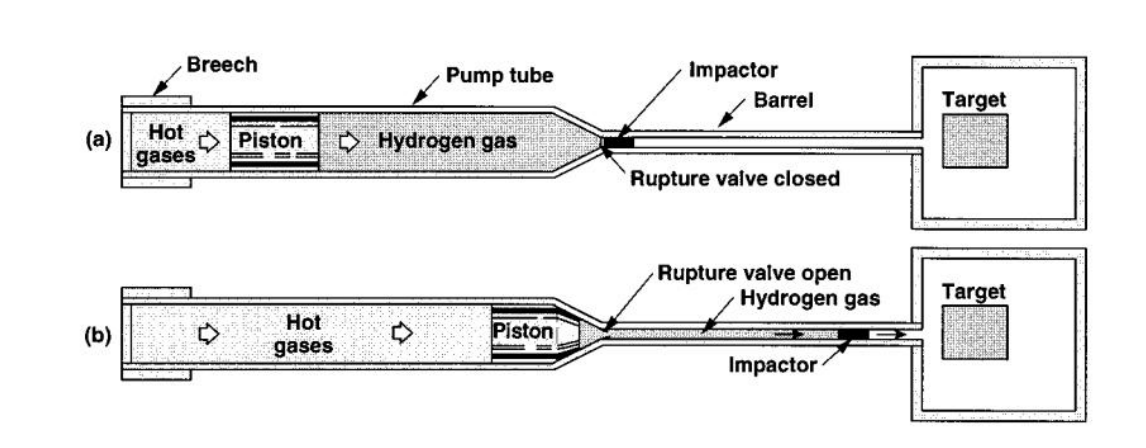
Questions: impact of other elements ?

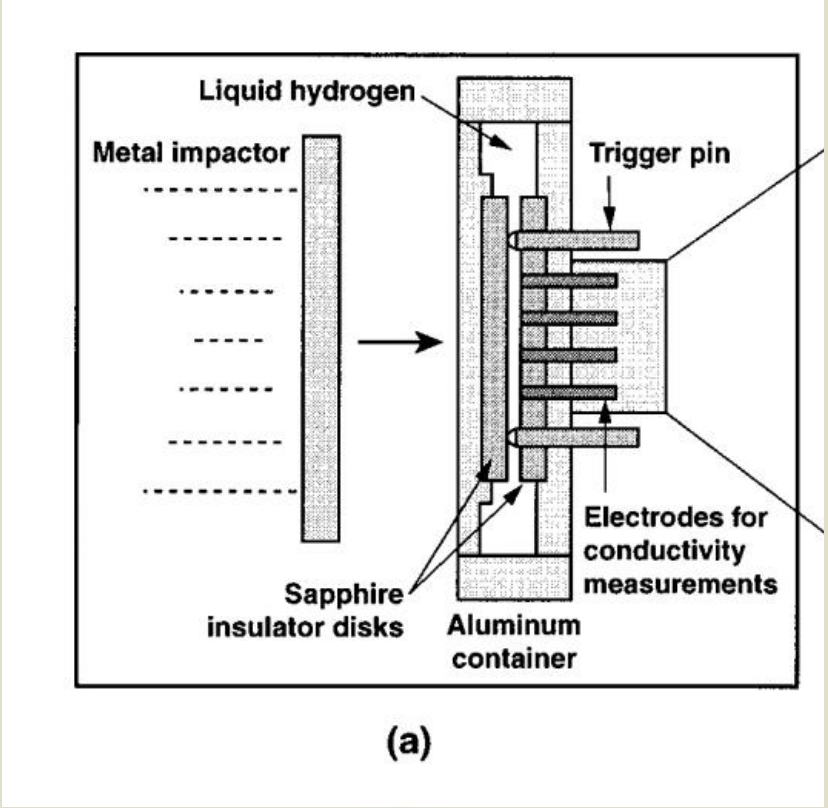


Zaghoo et al. 2016

II. Experiments

Conductivity measurements after « gun gas » shock





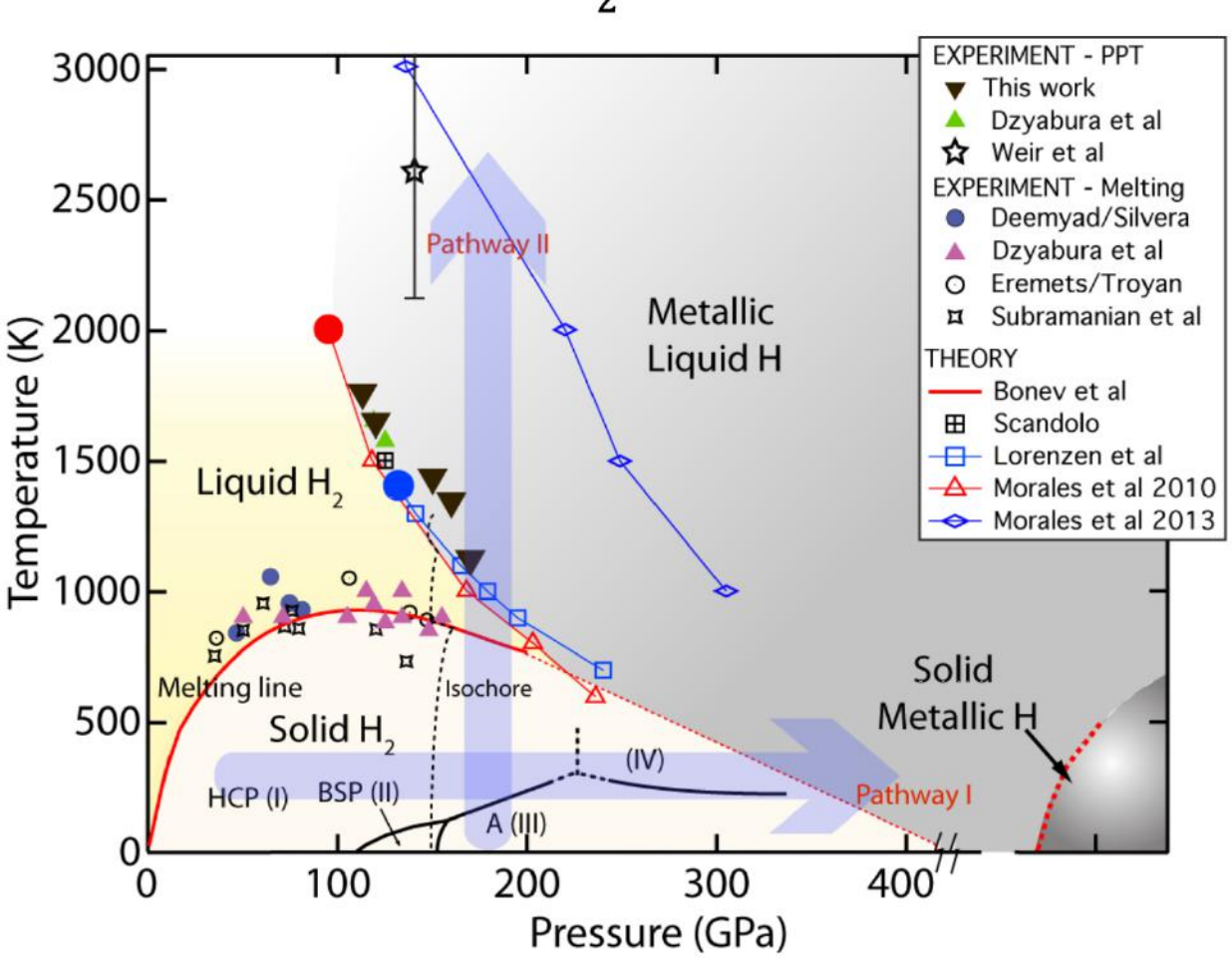
Nellis et al. 1999

II. Experiments

Zaghoo et al. 2016 (static)

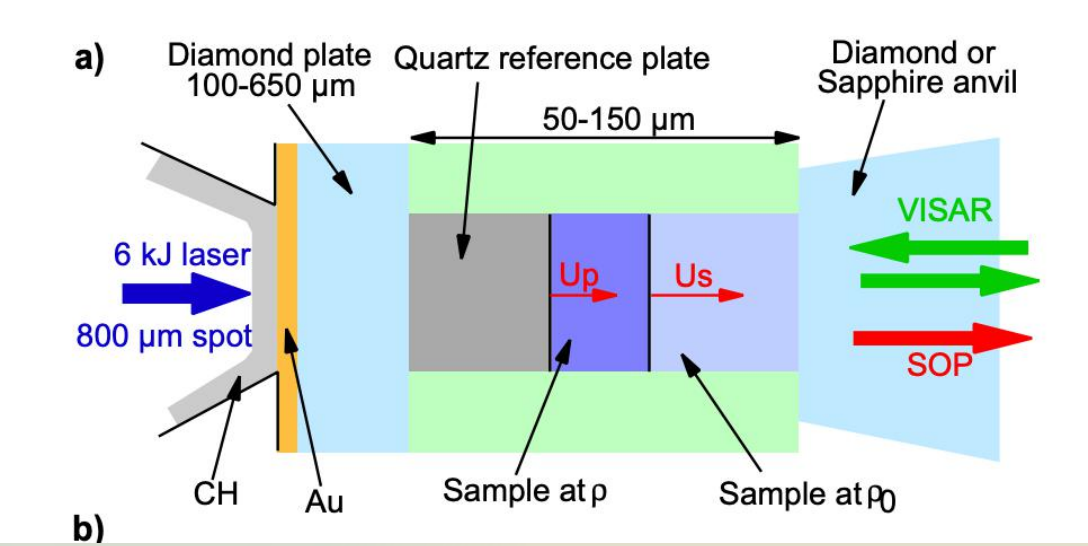
Celliers et al. 2018 (dynamic)

At least 3 reply each to criticize the methods



II. Experiments

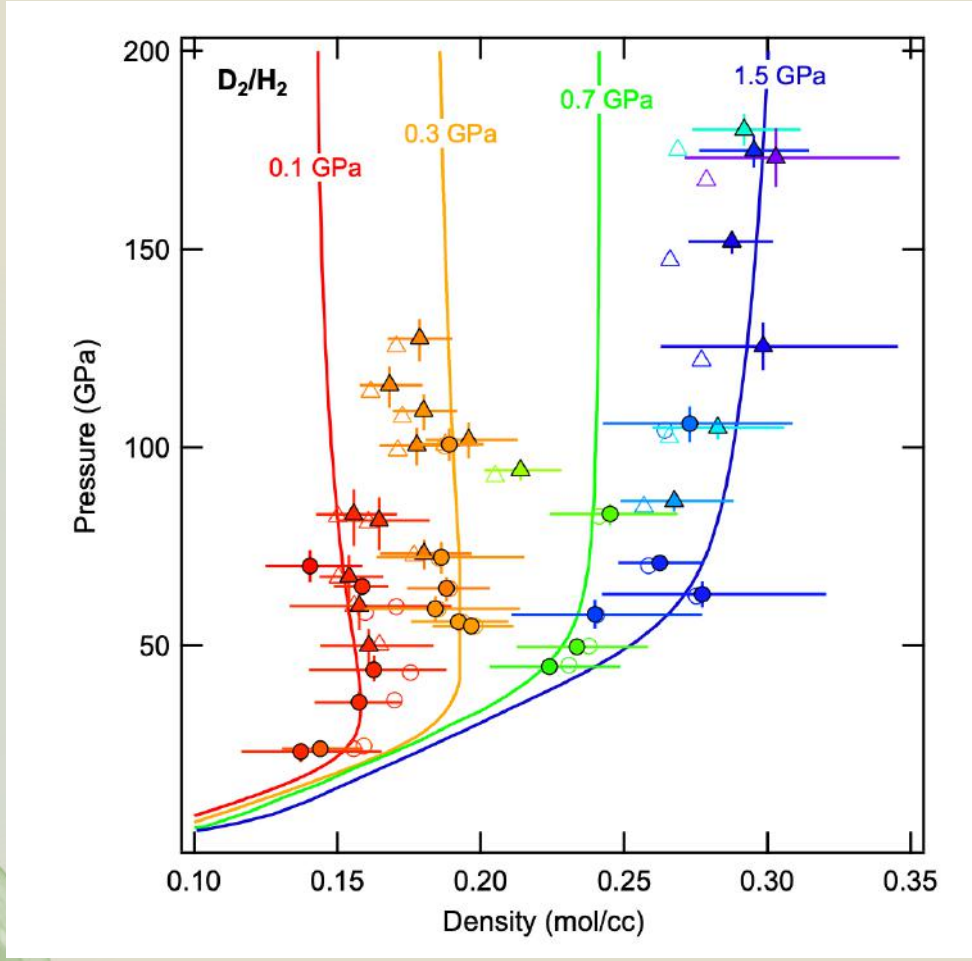
New method since ~ 2012: pre compressed dynamical compression



Brygoo et al. 2015

II. Experiments

Results:



Jupiter isentrope is obtained if the precompression is about 7 GPa. Coming soon.

II. Experiments

Summary: Goncharov 2020

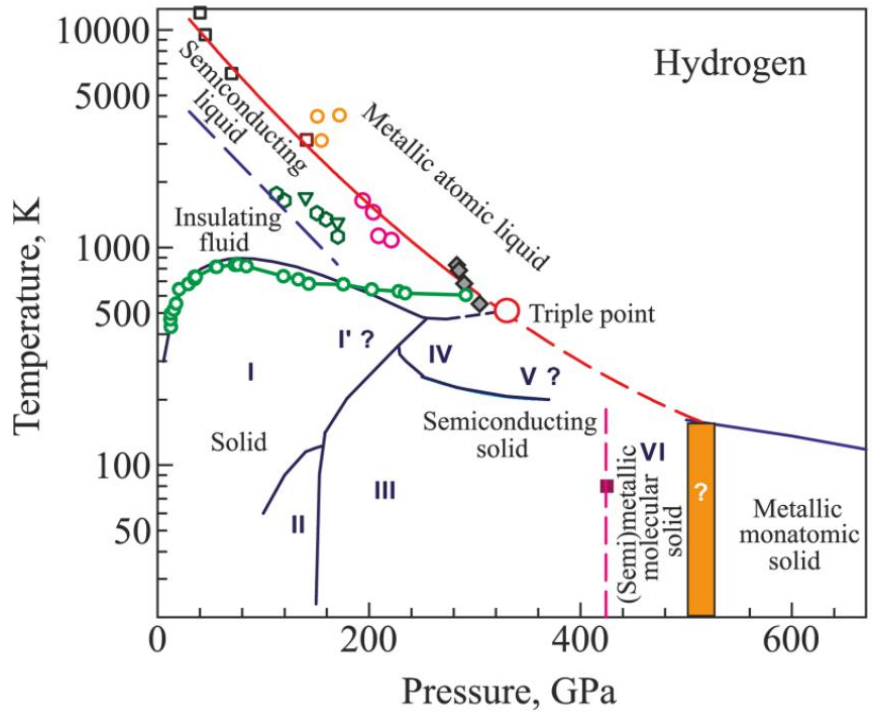


FIG. 1. Phase diagram of hydrogen at high pressures and various temperatures. The solid dark blue lines are the phase lines between the solid molecular phases and the melt line from Refs. 33–35 and the dashed line is the extrapolation of the melt line to higher pressures. An alternative and substantially different set of measurements of the melt line by Zha *et al.*[36] is depicted by open green circles and solid green lines. A solid pink square corresponds to an IR bandgap closure reported by Loubeyre *et al.*[21] A vertical dashed pink line is a proposed associated phase line between a semiconducting and semi(metallic) molecular phase also probed via the electrical conductivity by Eremets *et al.*[24] A hypothetic transition to an atomic metallic phase is shown by an orange box. At higher pressure theory predicts an atomic metallic phase with a declining melt line shown by a solid blue line.[37] At high temperature, the experiments and theory show two almost parallel boundaries corresponding to a transition into a semiconducting state (dashed blue line) and insulator-metal transition (solid red line). These have been measured by direct and indirect DAC and dynamic compression techniques.[38–45] Green symbols correspond to the DAC reflectance measurements in a pulsed laser-heated DAC,[46,47] which disagree with other DAC pulsed laser heating reflectance experiments shown by open orange circles.[29] Open black squares are from laser shocks,[43] open pink circles are from laser-driven ramp compression,[42] and grey diamonds are the Z-machine dynamic data,[41] which were temperature corrected in Ref. 42.

II. Experiments

Globally: we are getting to the conditons of giant planets

Lots of debate in the community, no consensus

Precompressed dynamic observations are the most promising avenue today

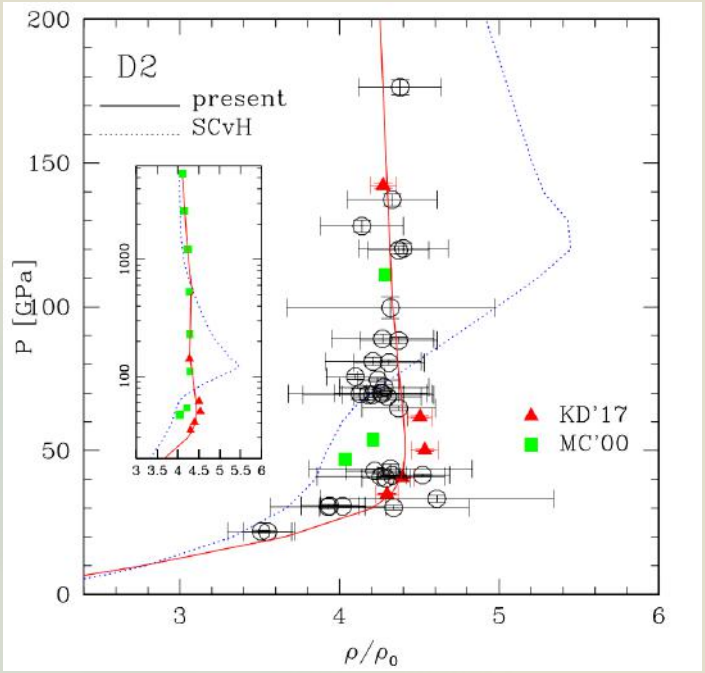
III. Comparison with EOS

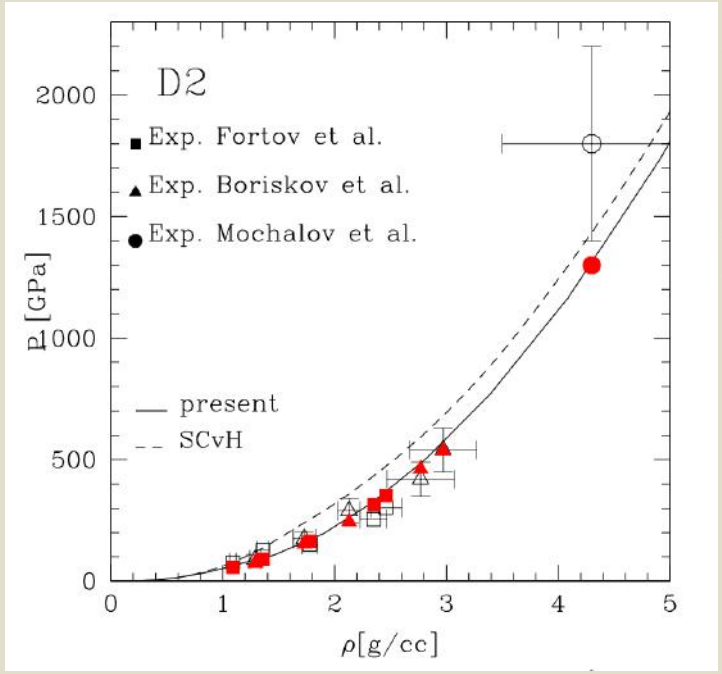
Known for 10 years: SCvH is no more accepted

First big improvement: MH13, non ideal H-He effects.

Improvement of the ionisation of H + gathering of simulations: Chabrier, Mazevet and Soubiran 2019.

III. Comparison with EOS

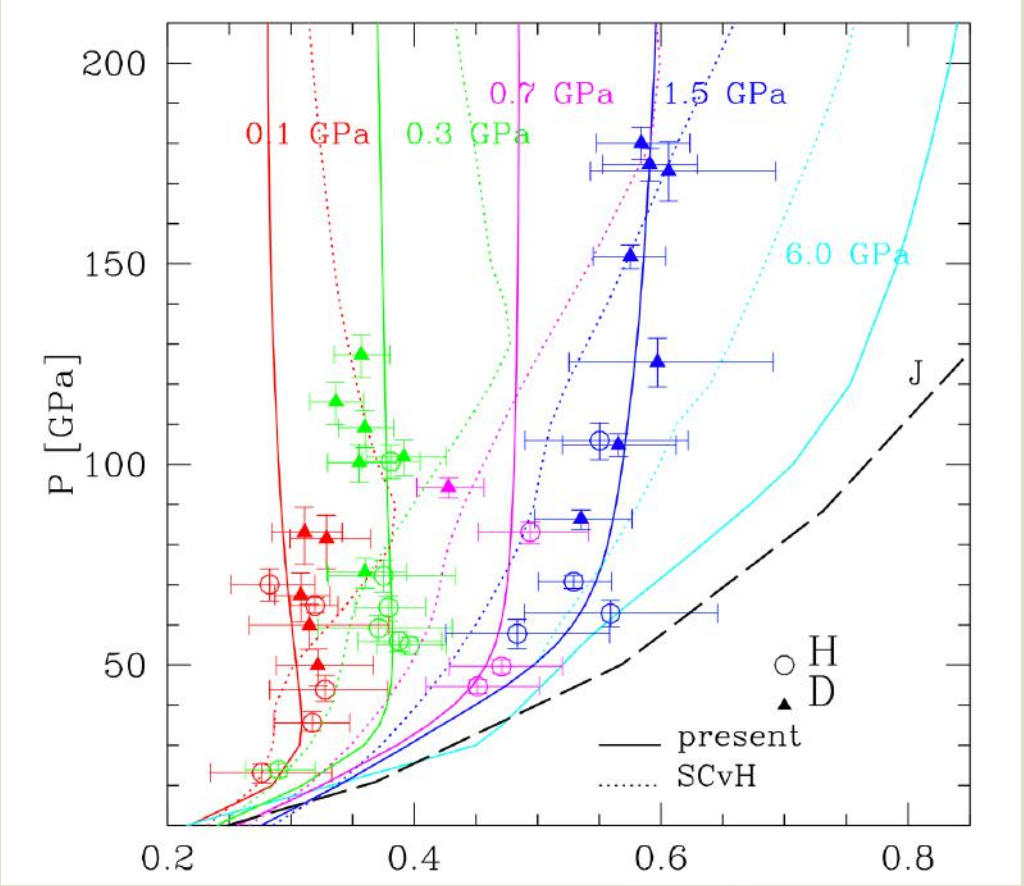




III. Comparison with EOS

Fits well the most recent experimental data on H and D

Almost at Jupiter's external isentrope

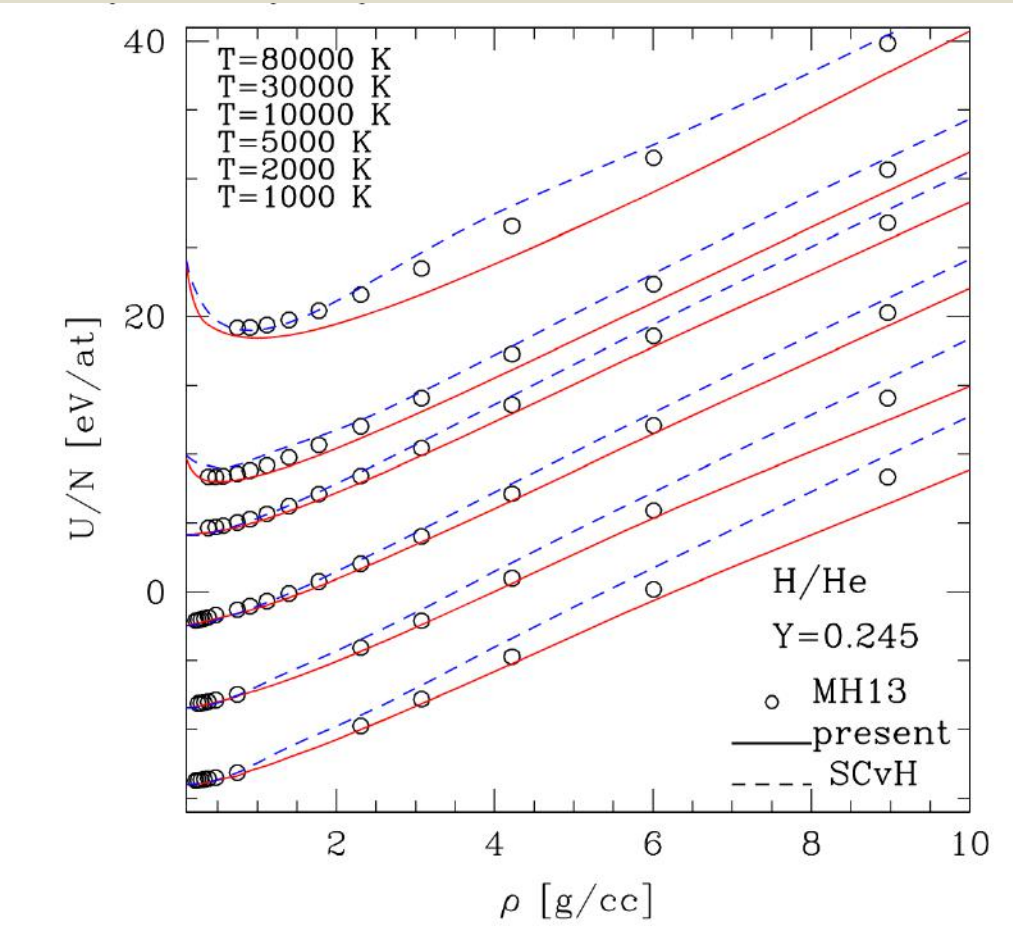


III. Comparison with EOS

Works also very well with He

BUT

not with H-He



III. Comparison with EOS

Idea from Miguel et al. 2016:
Non ideal terms included in a « pseudo » H EOS

Additive volume law, not valid in the non ideal case, states:

$$\frac{1}{\varrho} = \frac{X}{\varrho_H} + \frac{Y}{\varrho_{He}} \text{ and } S = XS_H + YS_{He} + S_{mix}$$

III. Comparison with EOS

Assume that our He EOS is perfect, and that non ideal terms can be incorporated in a modified H EOS.

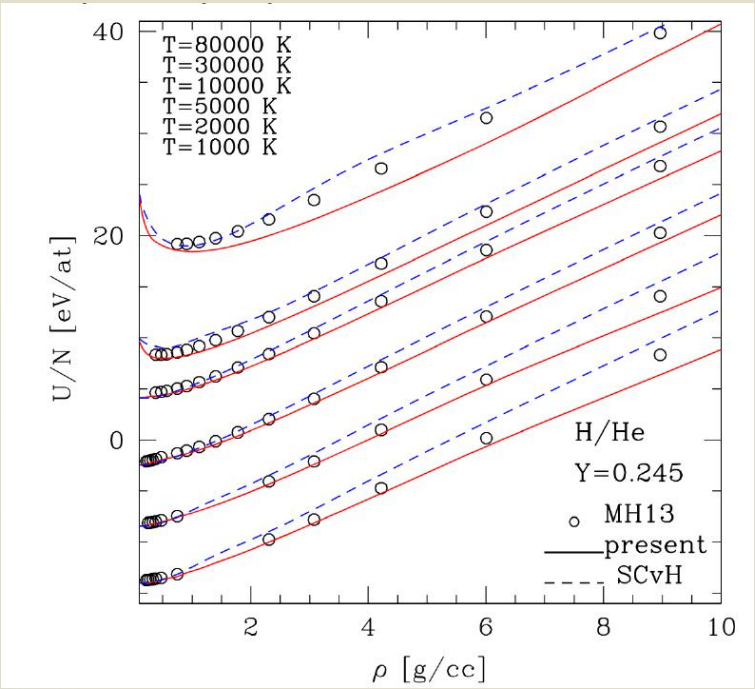
We just need to fit our new H EOS to recover the simulation results (MH13) under the additive volume law:

$$\frac{1}{\varrho_{H,new}} = \frac{1}{X_{MH13}}\left(\frac{1}{\varrho_{MH13}} - \frac{Y_{MH13}}{\varrho_{He}}\right) \quad and \quad S_{H,new} = \frac{1}{X_{MH13}}(S_{MH13} - Y_{MH13}S_{He} - S_{mix})$$

III. Comparison with EOS

We now have a new EOS, with non ideal effect artificially taken into account with a modified AVL.

Not yet at the 1% level Required by Stevenson



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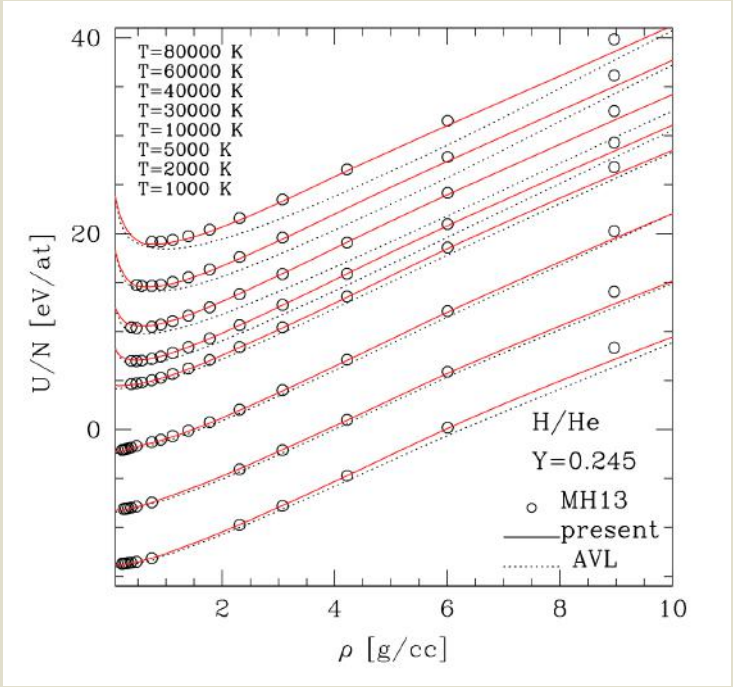

Chabrier & Debras 2021

Conclusions

Simulations: QMD, DFT, PIMC

Improvements allows comparison, no consensus yet but getting to it.
Prediction of metallisation, immiscibility

Experiments: dynamic, static, precompressed dynamic
Next generation representative of Jupiter. No mixture yet

EOS: knowledge of the behaviour of H-He allows predictions for giant planets and brown dwarves, although improvements still needed

Thank you !