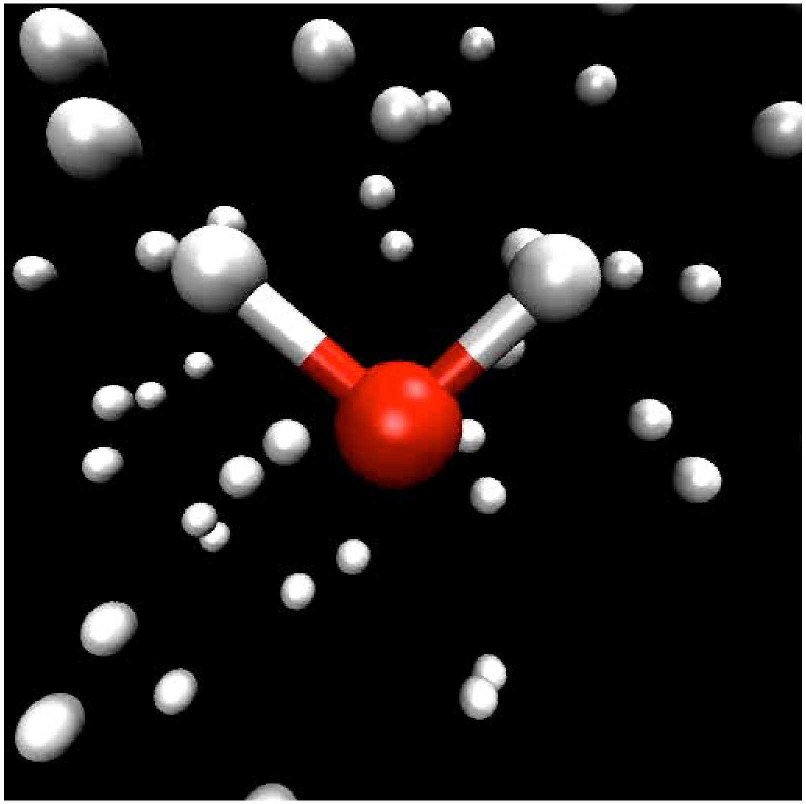
Understanding the Interiors and Evolution of Giant Planets Through First-Principles Computer Simulations



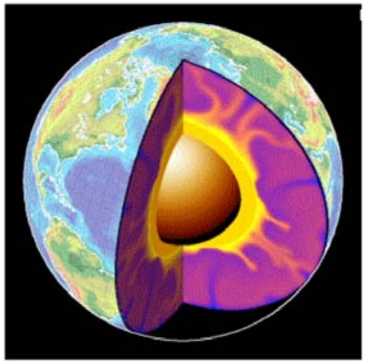
Burkhard Militzer

May 23, 2007

Geophysical Laboratory

Carnegie Institution of Washington

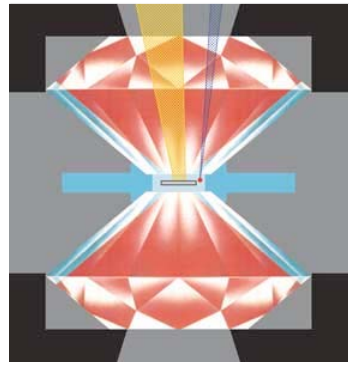
http://militzer.gl.ciw.edu



Study earth materials

High pressure experiments

Now also astrobiology



Diamond anvil cell exp.:

Ho-kwang Mao,

Russell J. Hemley

Original mission: Measure Earth's magnetic field (Carnegie ship)

Today: astronomy (Vera Rubin, Paul Butler,…) and isotope geochemistry

Outline and Acknowledgements

Hydrogen-helium calculation:

Path Integral Monte Carlo (PIMC)

Density Functional Theory
Jan Vorberger (Carnegie Institution of Washington)
in collaboration with **I. Tamblyn, S. Bonev** (Dalhousie U.)

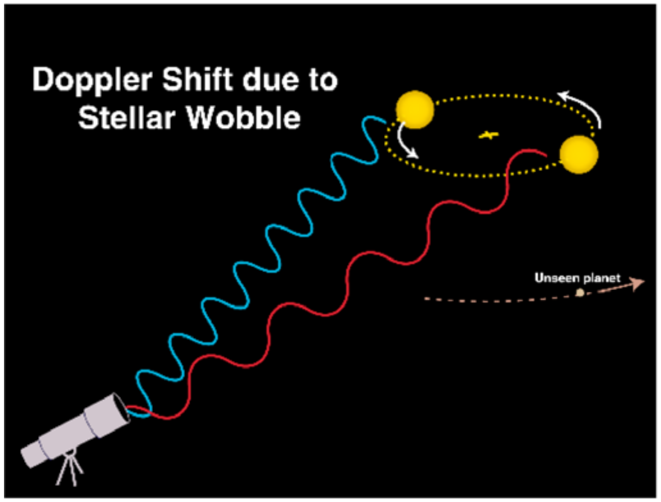
Modeling of Jovian planets:

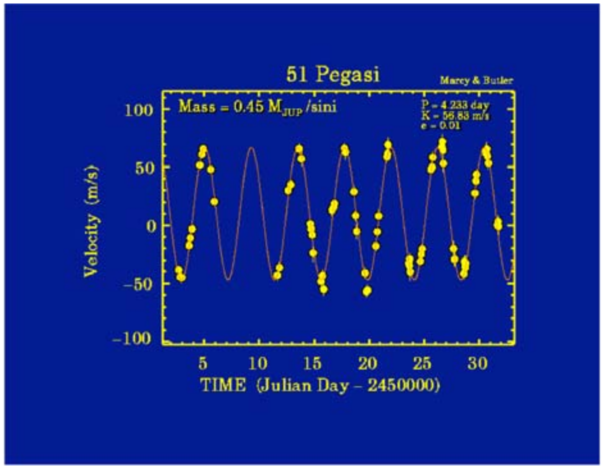
W. Hubbard (LPL, Arizona SU, Tucson)
David Stevenson (Caltech)

Supported by NASA under the grant NNG05GH29G, by the NSF under the grant 050732, and by the Carnegie Institution of Canada.

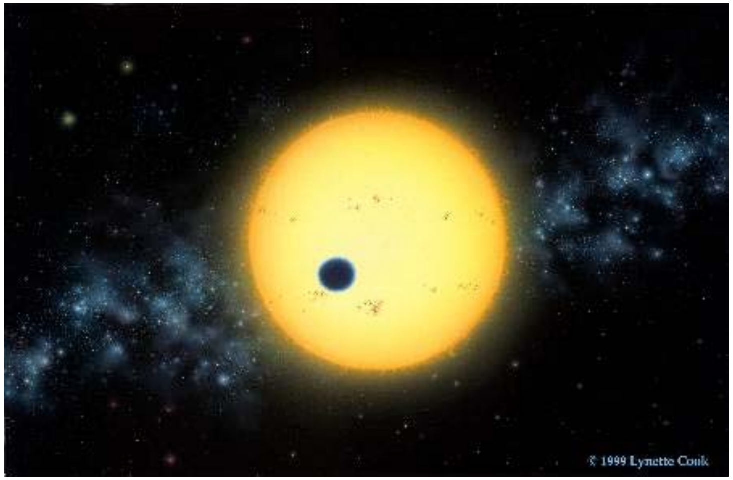
Detection Techniques for Extrasolar Planets: radial velocity technique, transient method, ...

200+ planets found with radial velocity meas.





14 planets seen with transient technique



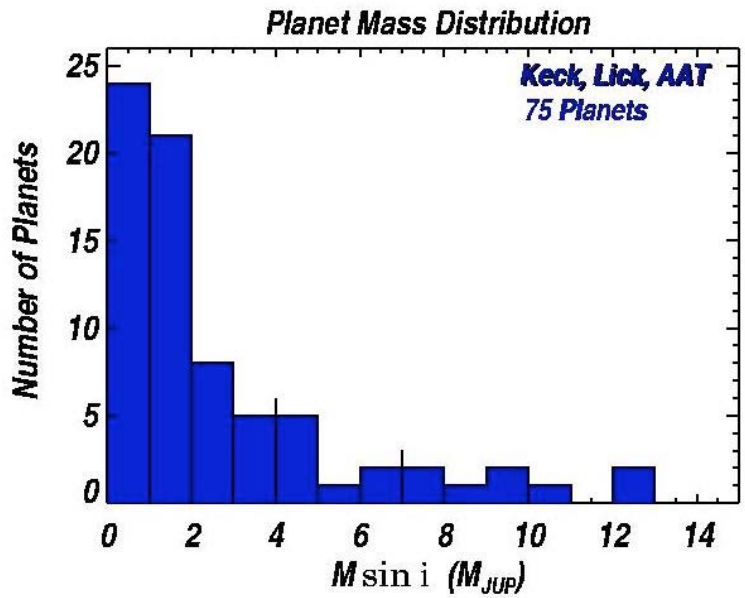
First planet detected:

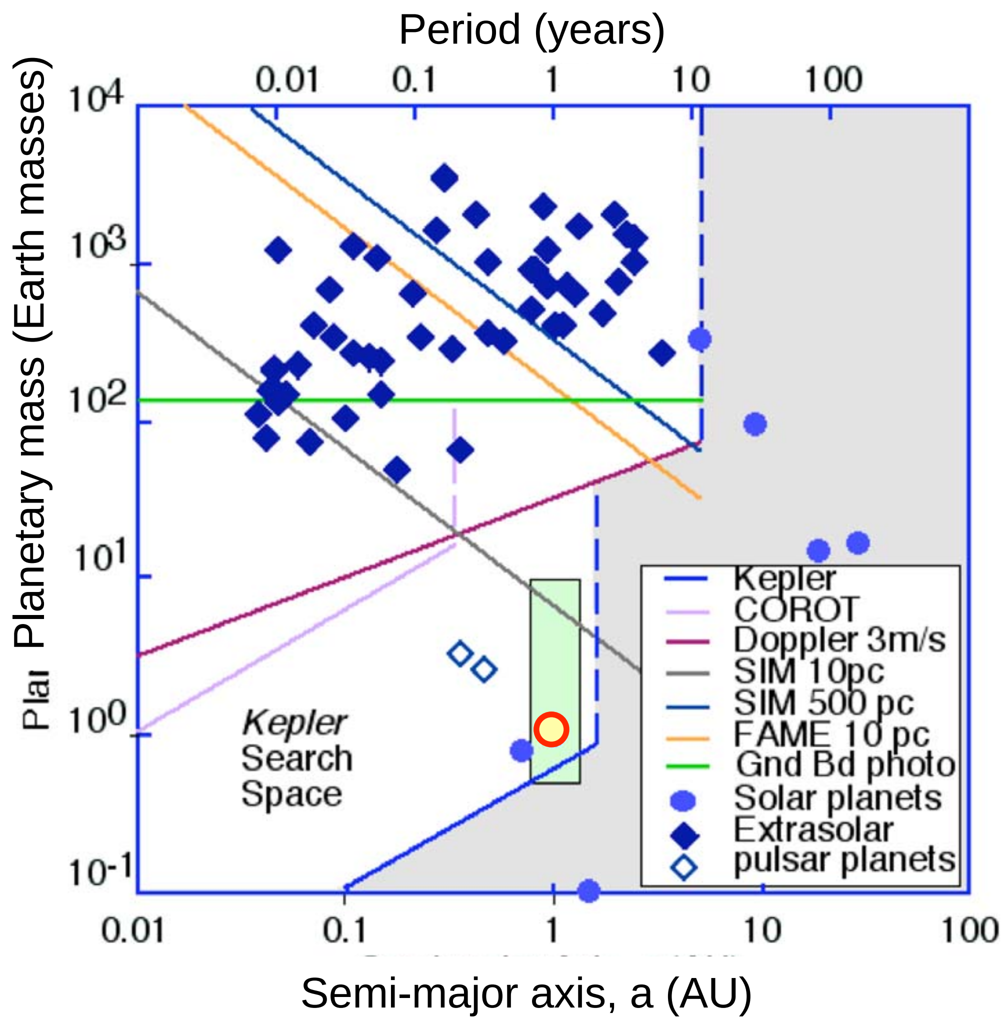
Mayor & Queloz, Nature 378 (1995) 355
(Geneva Observatory)

Orbital period: 4.23 days !
Msin(i) = 0.46
a = 0.05 AU

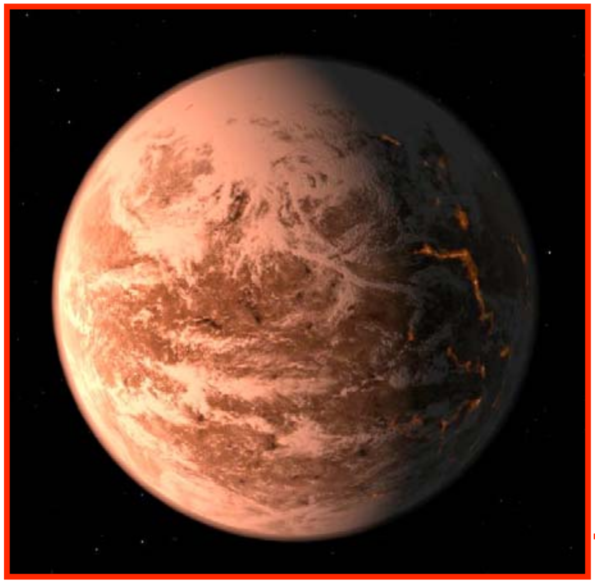
Characteristics of the 200+ known extrasolar planets

How far away are we from detecting an Earth like planet?

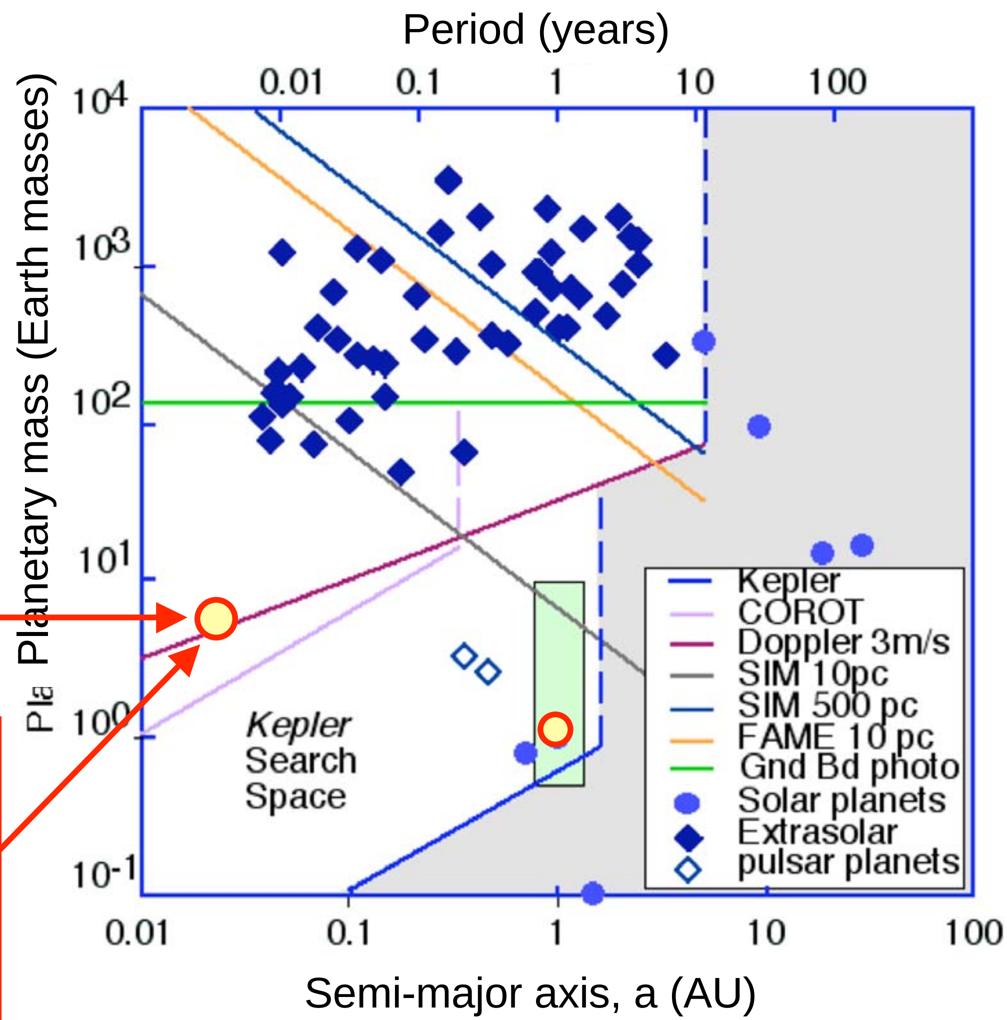




Light addition: a planet with only 7 Earth masses

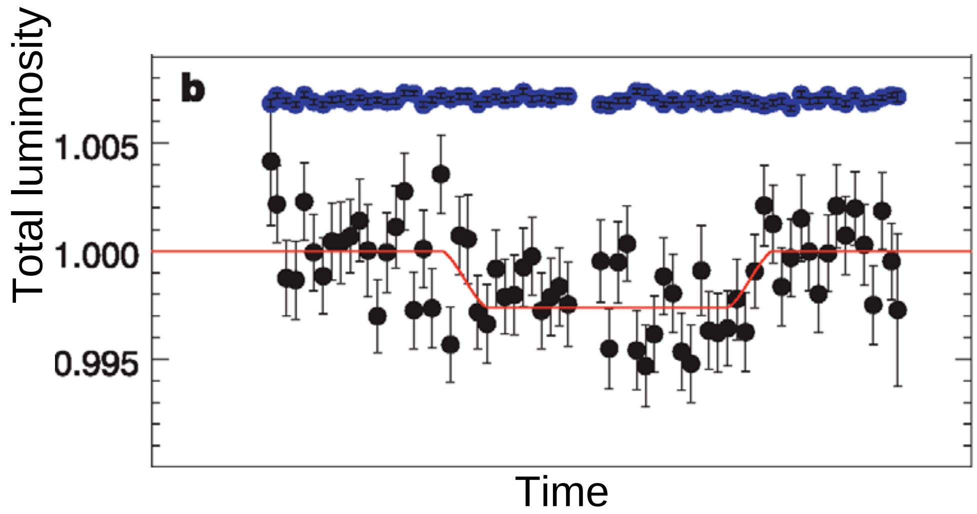


Trent Schindler (NSF)

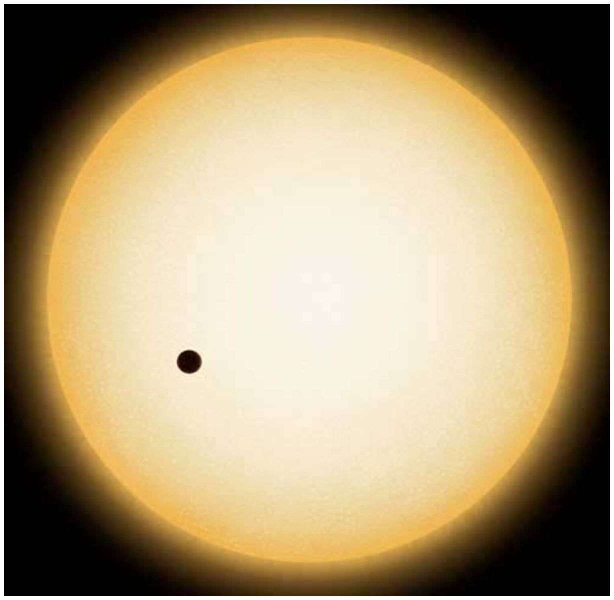


Planet of 6-8 earth-masses orbiting close to Gliese 876
[E.Rivera et al., ApJ 635 (2005) 625]
Orbital period: 1.94 days !
Msin(i) = 5.9 earth masses
a = 0.021 AU

Two very recent discoveries: 1) First observation of secondary eclipse 2) new transiting planet



Saturn-mass planet with large dense core transits across HD 149026 [B. Sato et al. ApJ, 633 (2005) 465].



Exoplanets.org

1) First observation of a secondary eclipse of a extrasolar plant:
Deming *et al.*, Nature 434 (2005) 740.
Charbonneau *et al.* Astrophys. J. (2005)

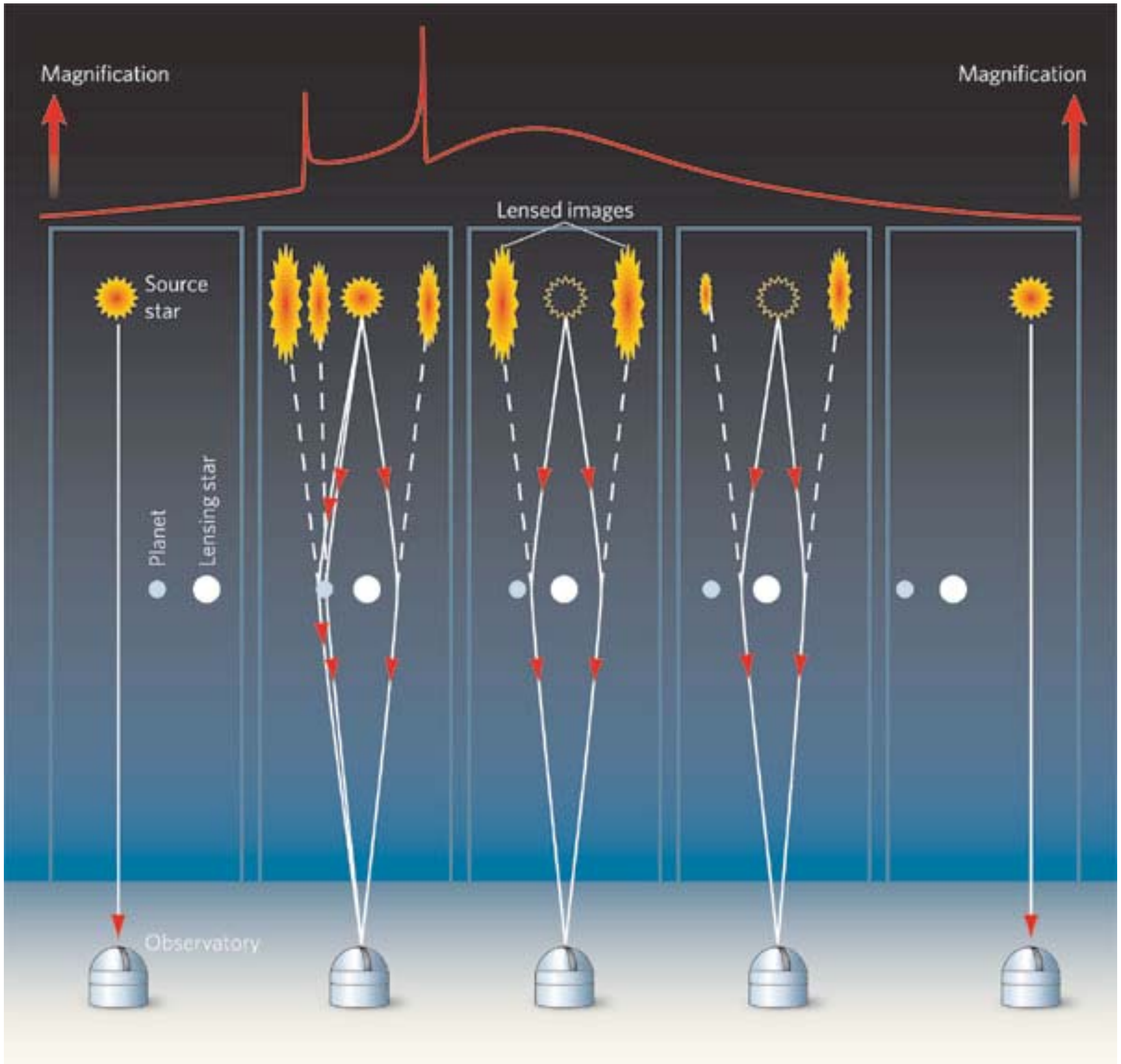
"Missing" light from planet can be characterized. Information about surface temperature and possibly composition.

2006: Third technique finds extrasolar planets: observation of gravitational microlensing events

So far, 4 planets found by observation of gravitational microlensing events.

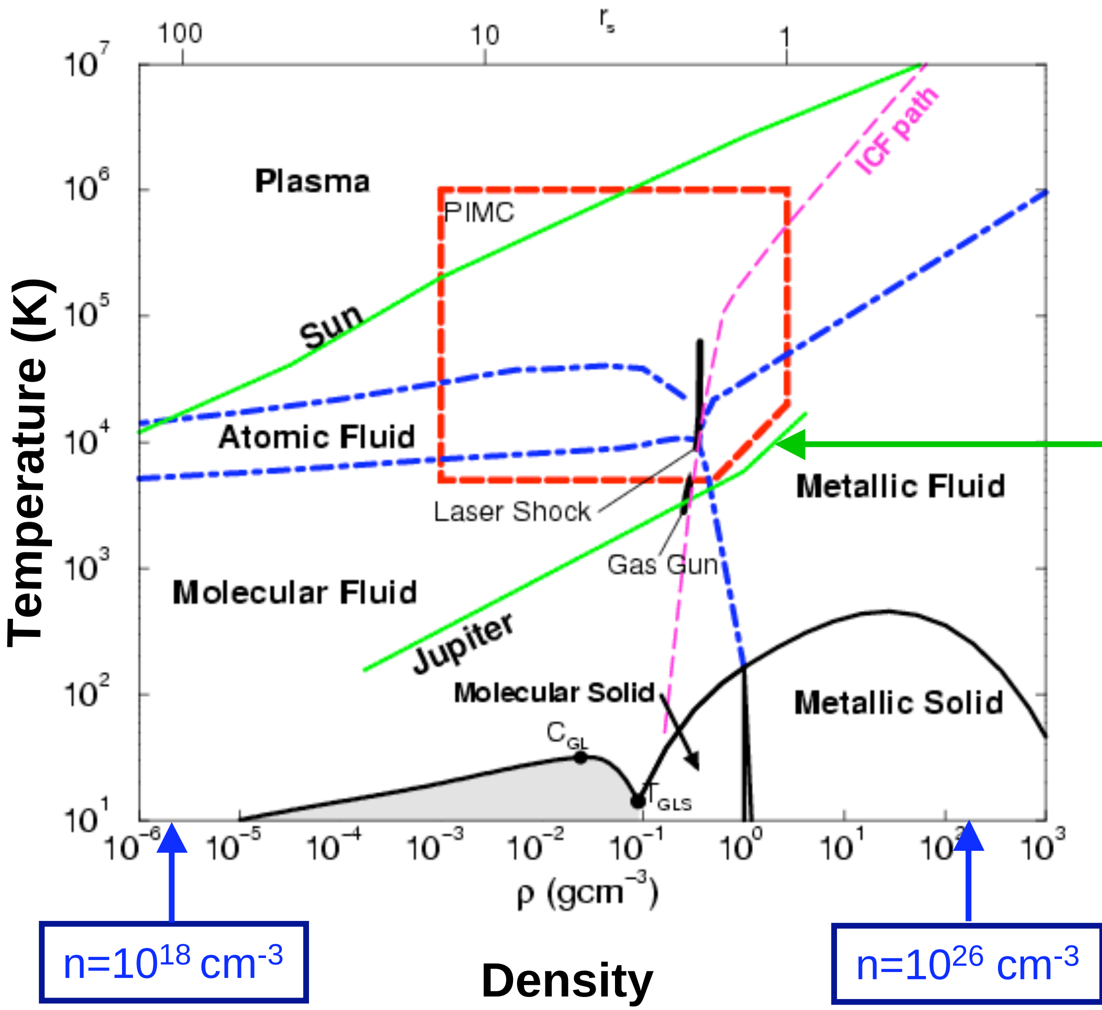
J.P. Beaulieu et al, Nature (2006).

Detected planet well below the Doppler detection limit.

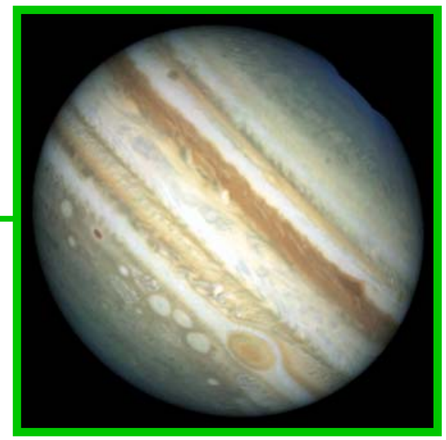


D. Queloz, Nature, New & Views (2006).

Focus: Characterization of the Interior of Solar and Extrasolar Giant Planets



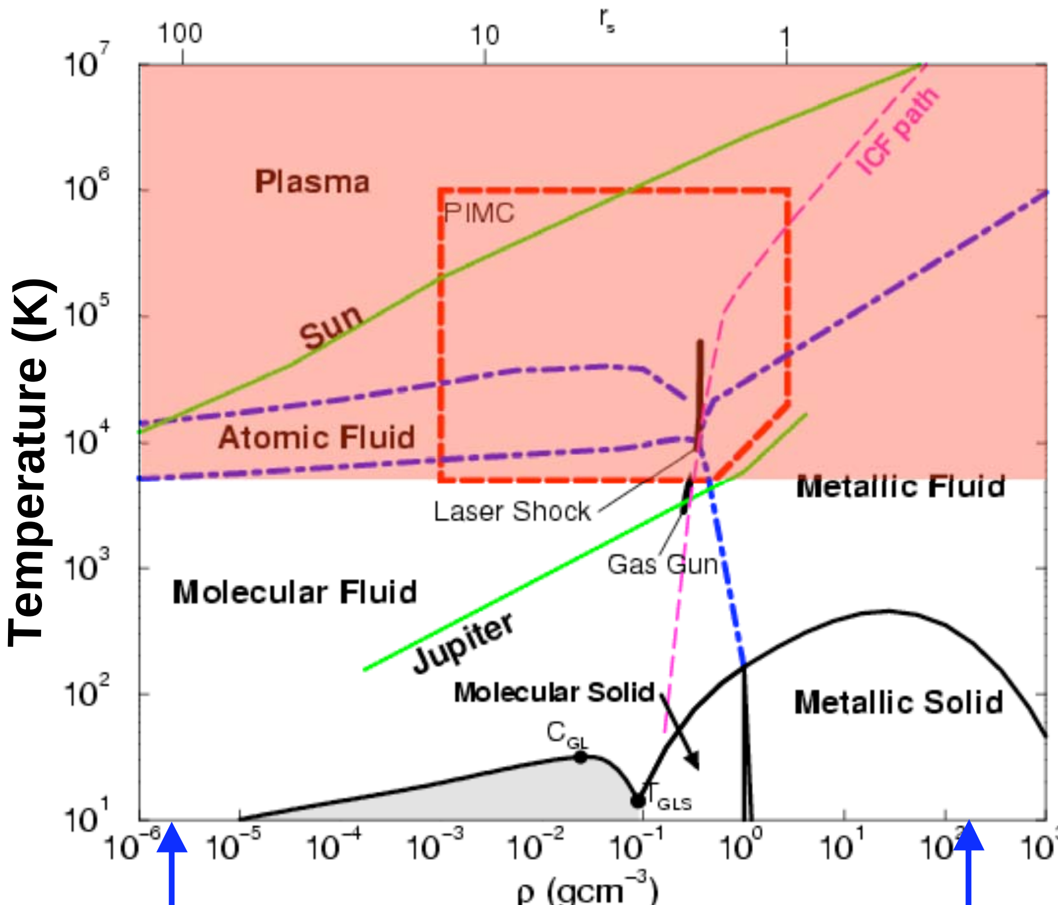
Solar GP: Jupiter, Saturn

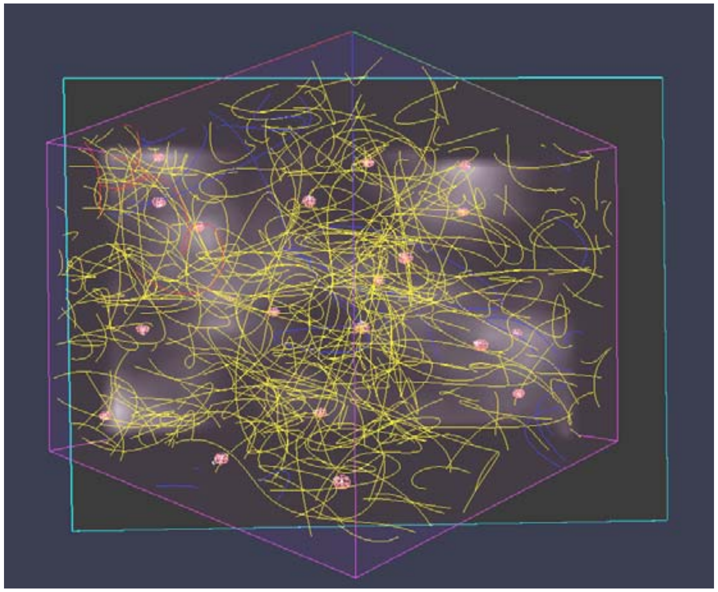


Paul Dirac (1929):

The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too ***complex to be solved*** ***`EXACTLY'*** [added by BM].

1) Path integral Monte Carlo for T>5000K



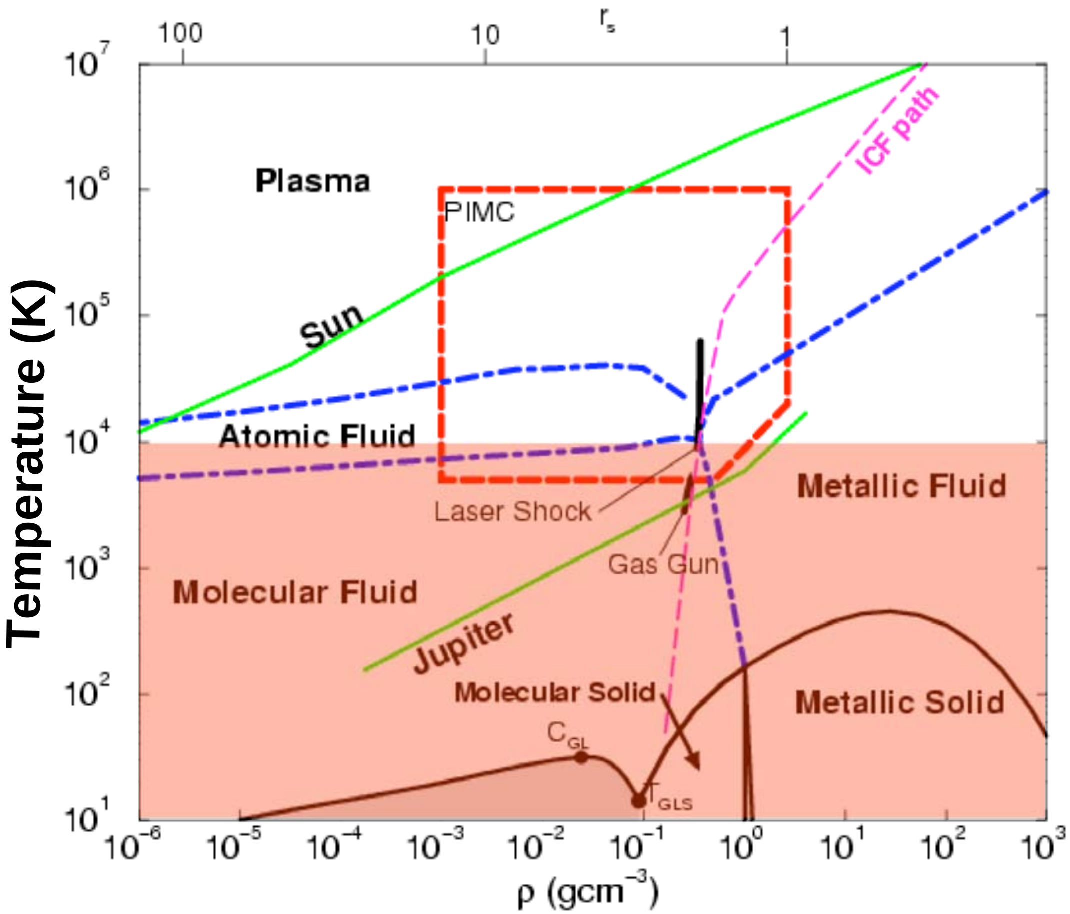


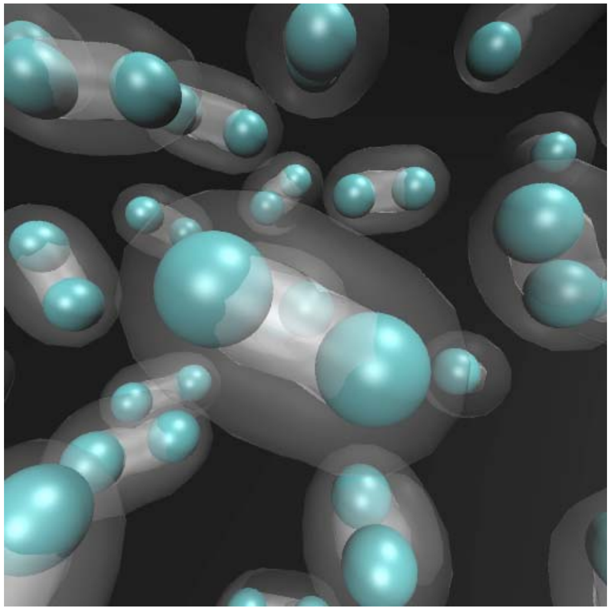
PIMC applicable at: T>5000K

n=10^{18} cm^{-3}

n=10^{26} cm^{-3}

1) Path integral Monte Carlo for T>5000K
2) Density functional molecular dynamics below



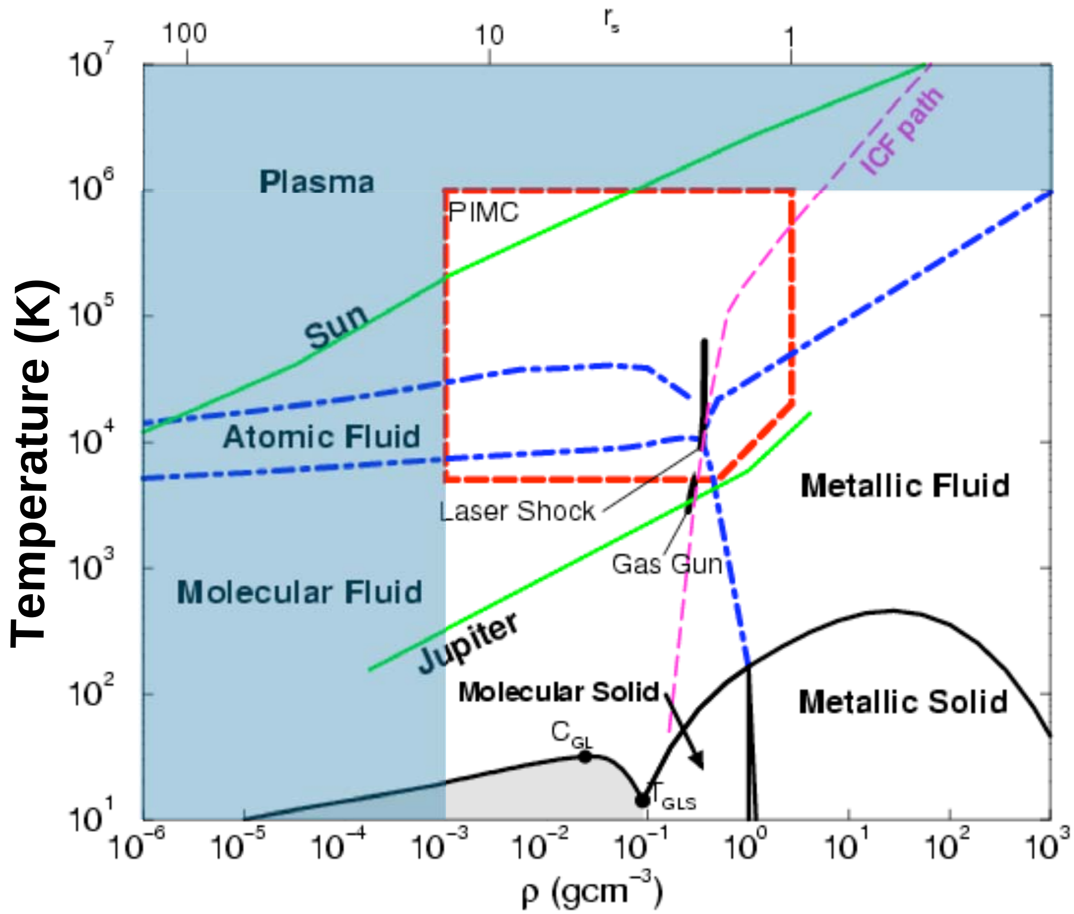


Born-Oppenheimer approx.
MD with classical nuclei:

F = m a

Forces derived DFT with electrons in the instantaneous ground state.

Use analytical (chemical) models at low density and very high temperature



Free energy model to describe weakly interacting chemical species:

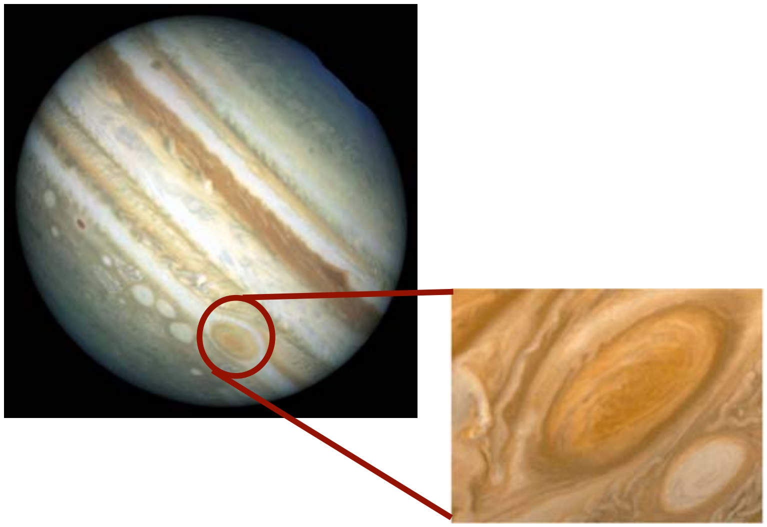
H_2, H, H^+, e^-

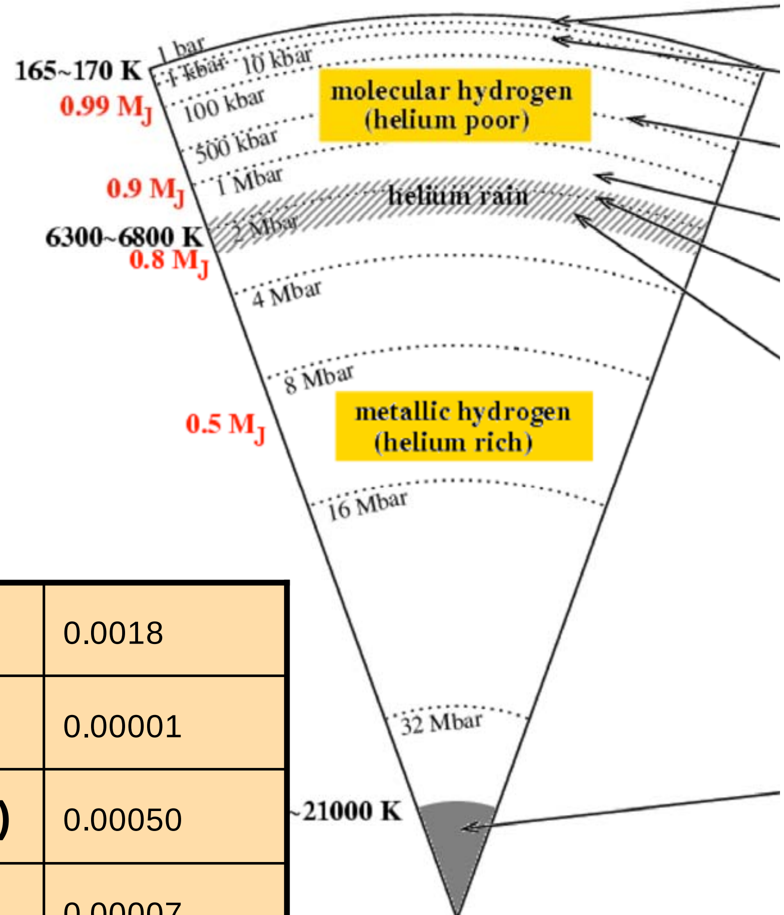
He, He^+, He^{++}, e^-

Free energy is constructed but it contains free parameters to describe the interaction.

- Saumon and Chabrier
- Sesame database
- Ross model

Jupiter is well characterized only on the surface.



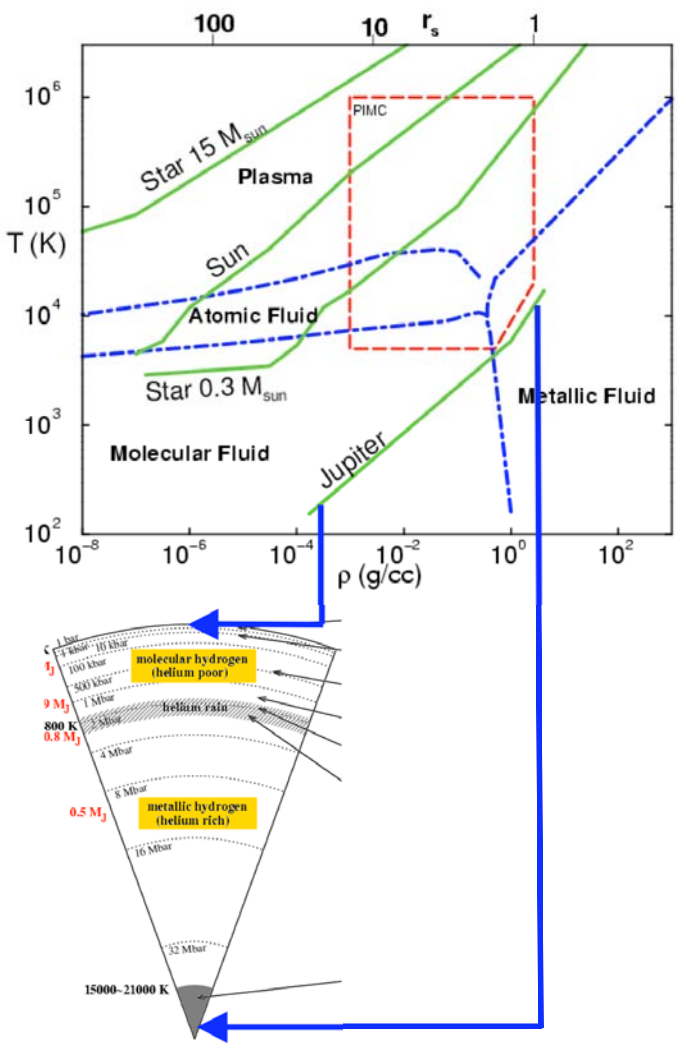


<u>Composition on the surface</u> <u>(solar):</u>

H	**0.742**	0.736	**Ne**	**< 0.0002**	0.0018
He	**0.231(4)**	0.249	**P**	**< 0.00007**	0.00001
C	**0.009(2)**	0.0029	**S**	**0.00091(6)**	0.00050
N	**< 0.012**	0.00085	**Ar**	**< 0.00015**	0.00007
O	**< 0.0035**	0.0057	**"Z"**	**0.027**	0.015

Guillot et al. (Jupiter book, 2002, chap.3)

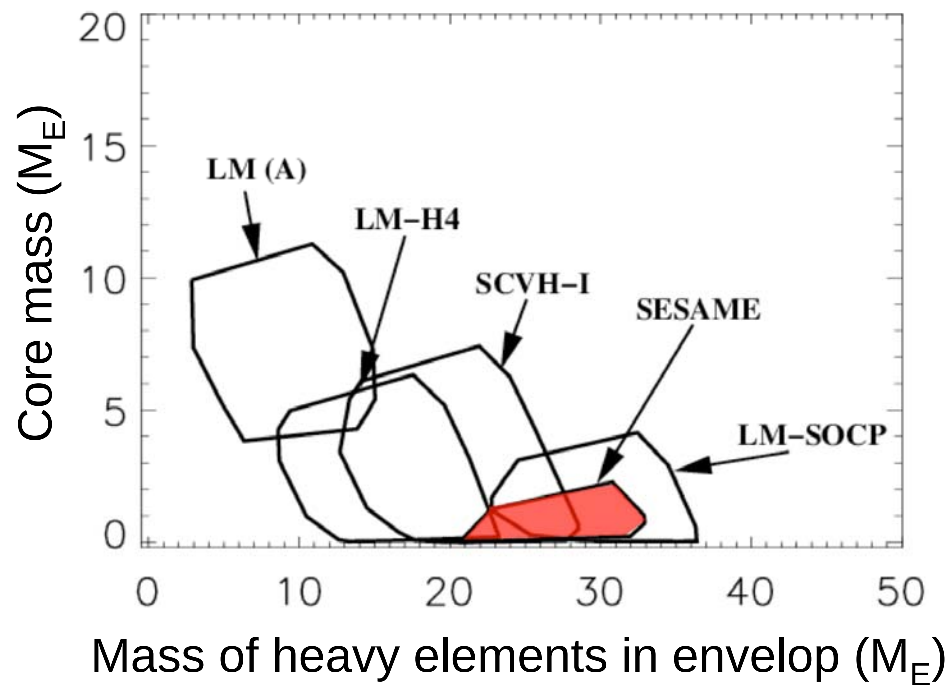
1. Guillot's model: Uncertainties in EOS do not allow to determine if Jupiter has a rocky core



T. Guillot's three layer model is based on

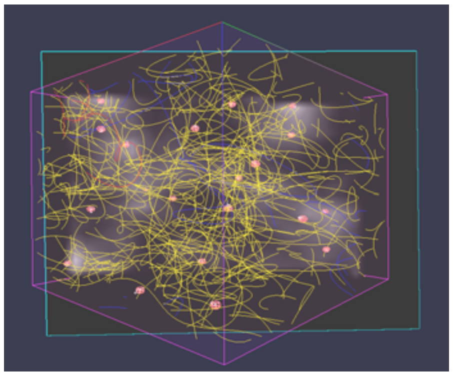
1) Hydrogen-helium EOS
2) Surface composition
3) Gravitational moments inferred from fly-by trajectories (Cassini mission)

Parameters like core mass or amount of heavier

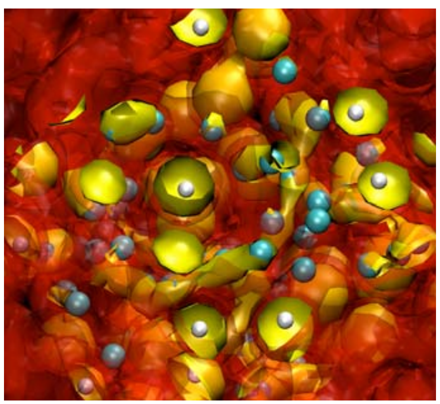


Two simulation techniques combined to study planetary interiors:

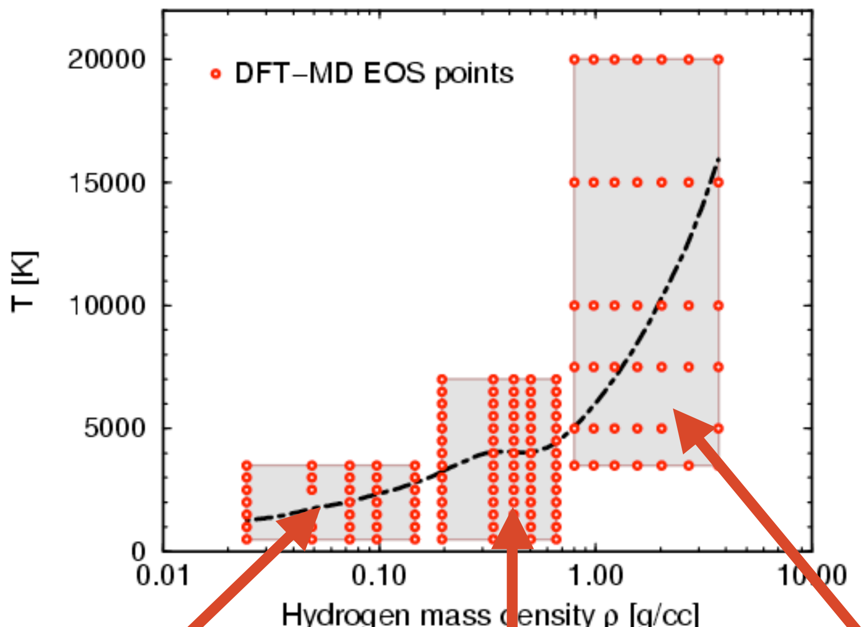
Path integral Monte Carlo and Density functional molecular dynamics

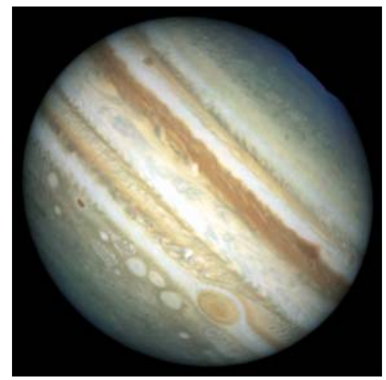


PIMC



DFT-MD



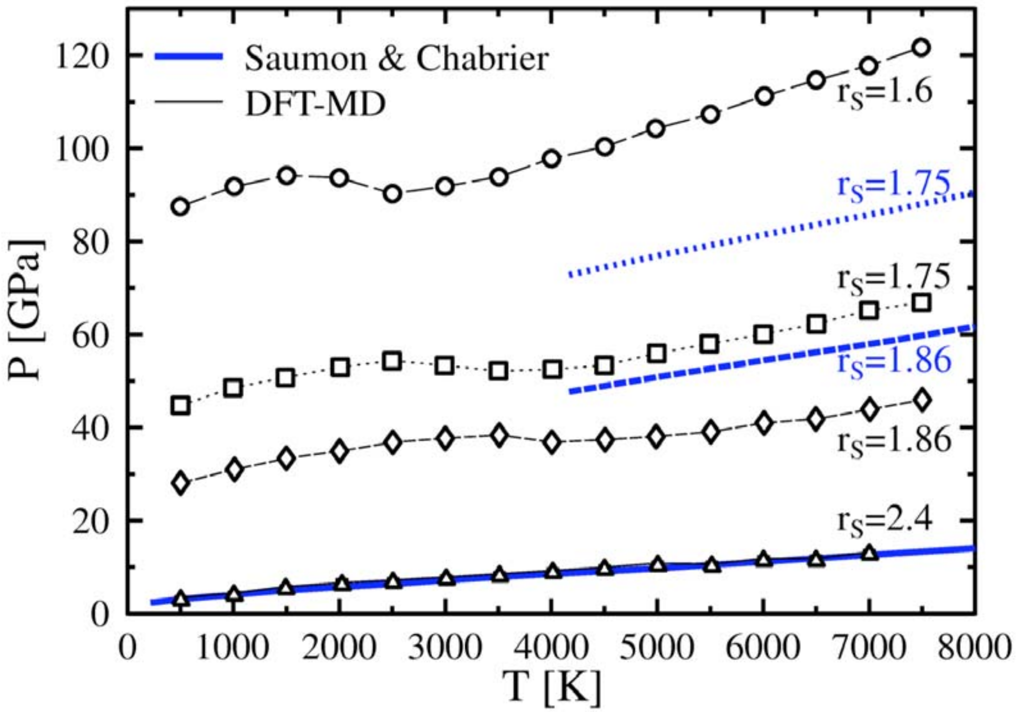


Molecular hydrogen

Transition region

Metallic hydrogen

Hydrogen EOS derived from DFT simulations

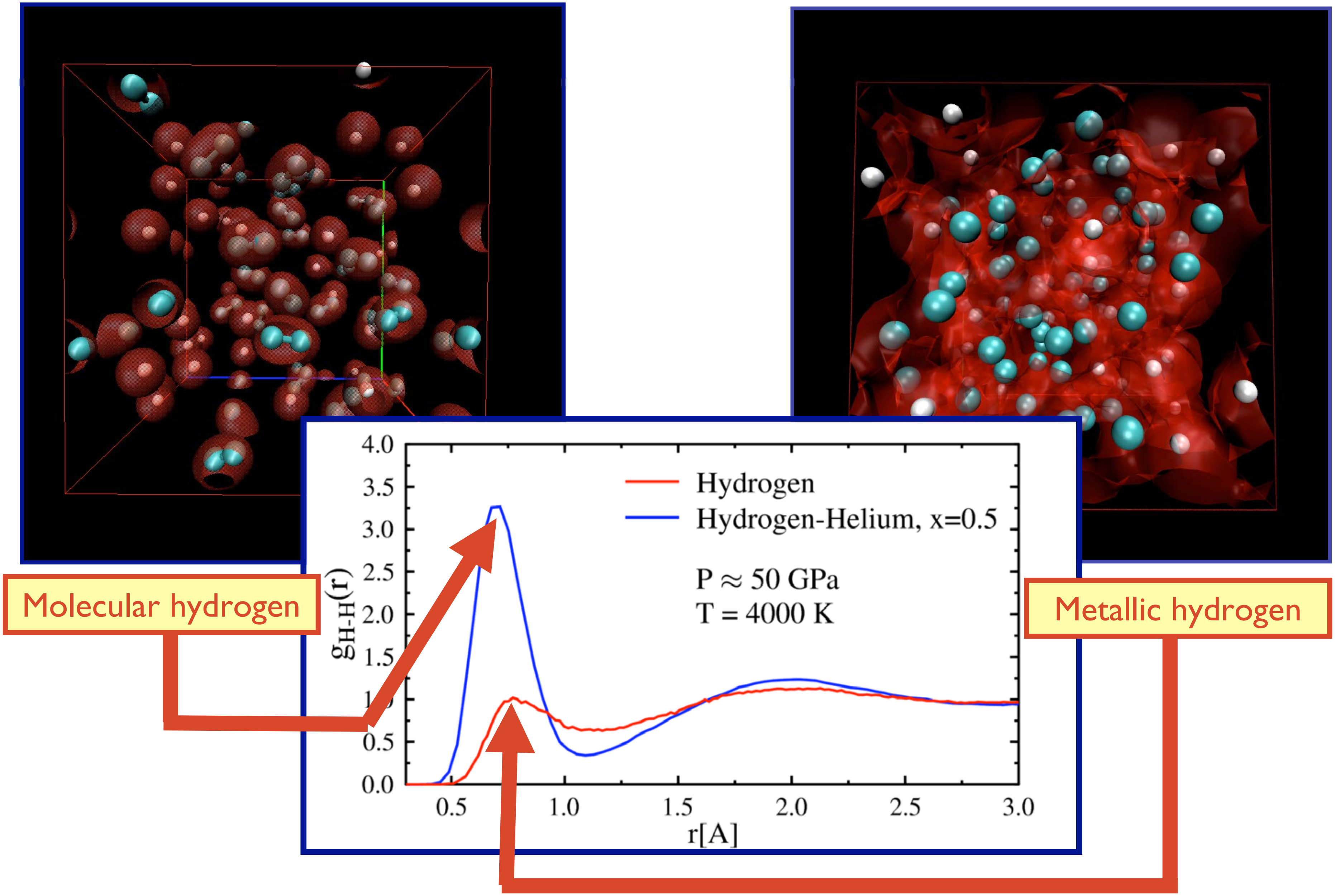


- Molecular to atomic transition is continuous as function of T (must use BOMD not CPMD)
- Negative $dP/dT|_V < 0$ region for pure hydrogen
- No such region H-He mixtures

In dissociation region, deviations from S&C of up to 20%.

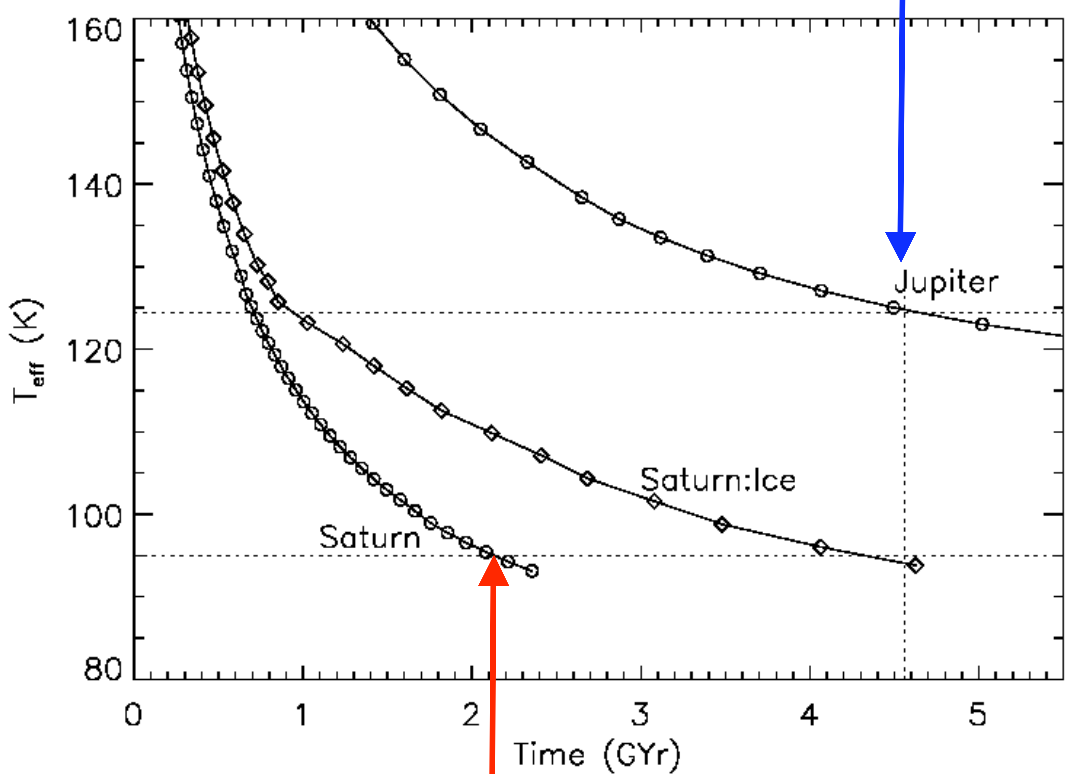
J. Vorberger, I. Tamblyn, B. Militzer, S. Bonev, "Hydrogen-helium mixtures in the interior of giant planets", *Phys. Rev. B* **75** (2007) 024206.

Simulations show that helium stabilizes H_2 molecules



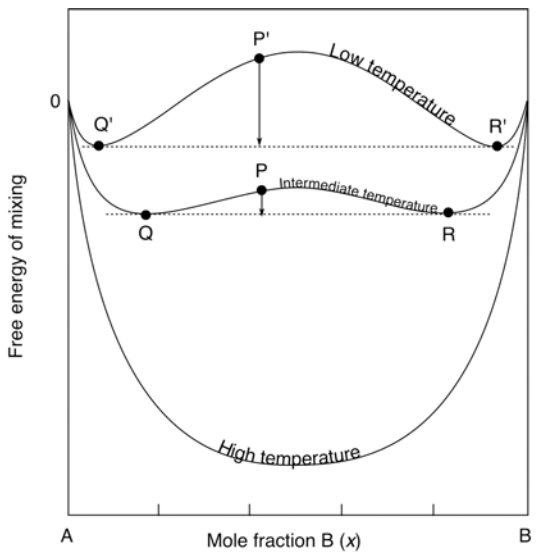
J. Fortney & W. Hubbard model the evolution of Jupiter and Saturn [Icarus, 2003]

Jupiter's cooling rate is in agreement with model predictions



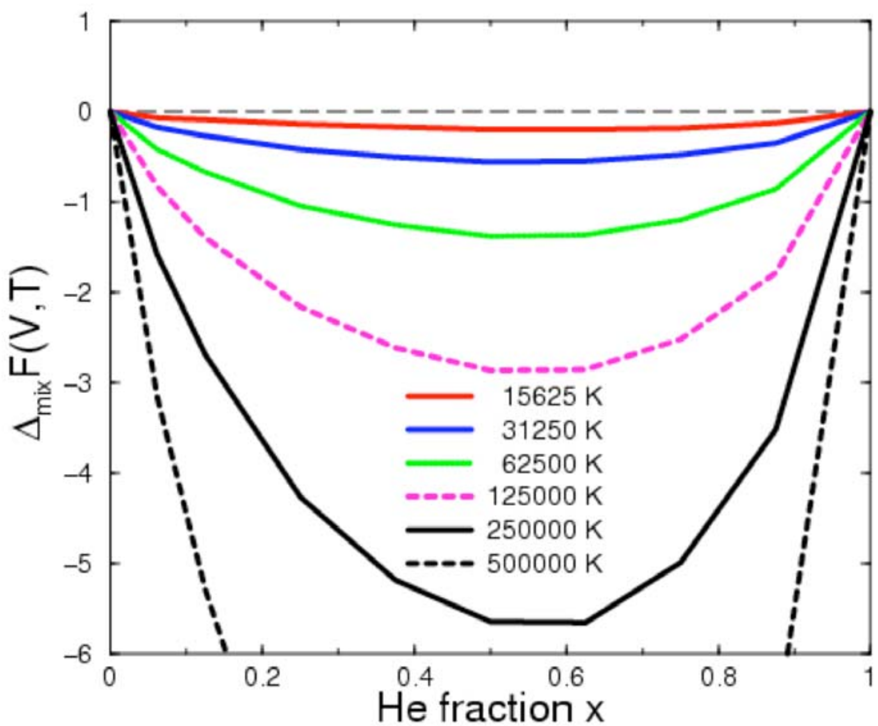
Model for Saturn consistently predict too fast cooling rates (by ~2 Gyrs)

Preliminary PIMC results for the mixing free energy



Mixing free energy $\Delta F_{mix}(V,T)$:

$$\Delta F_{mix}(x) = F(x) - x\,F(1) - (1-x)\,F(0)$$

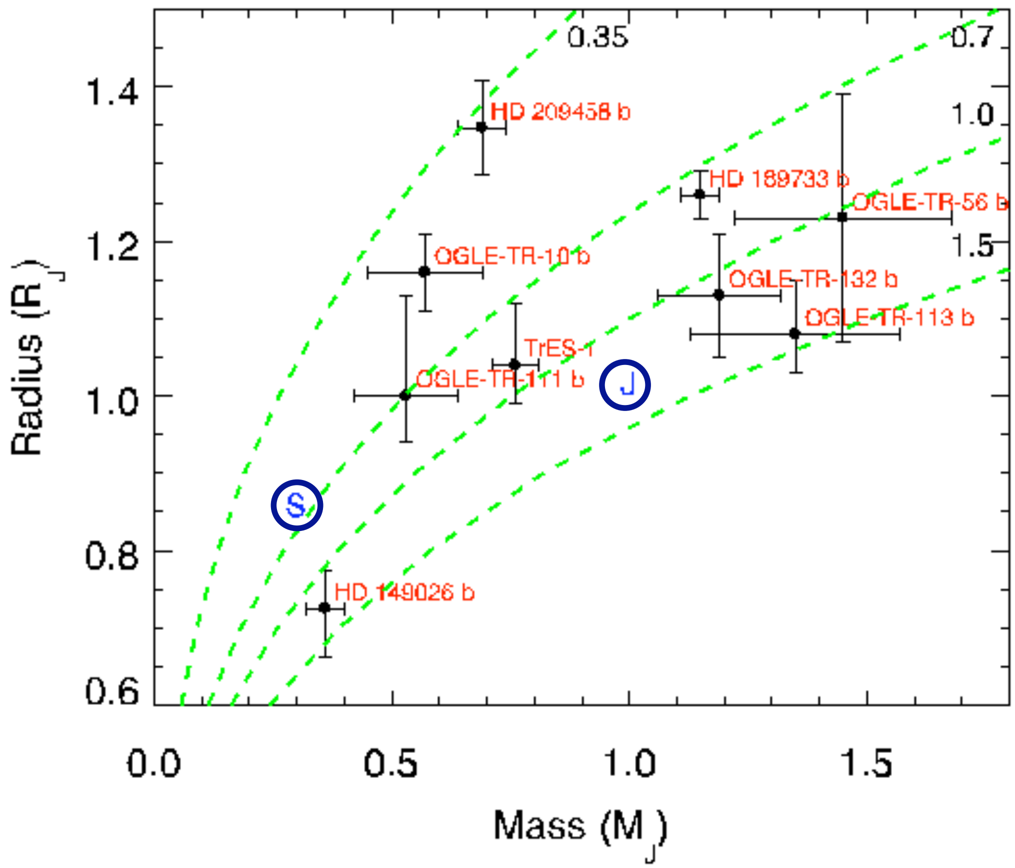


Difficulty to compute the Gibbs free energy of mixing G(ρ,T,x):

- Estimate ΔG by swapping particles (Bennett method)
- Thermodynamic integration over charge or over T.

Extrapolation predict demixing at about 8000K.

Mass-Radius Relationship of Recently Discovered *Transiting* Extrasolar Planets

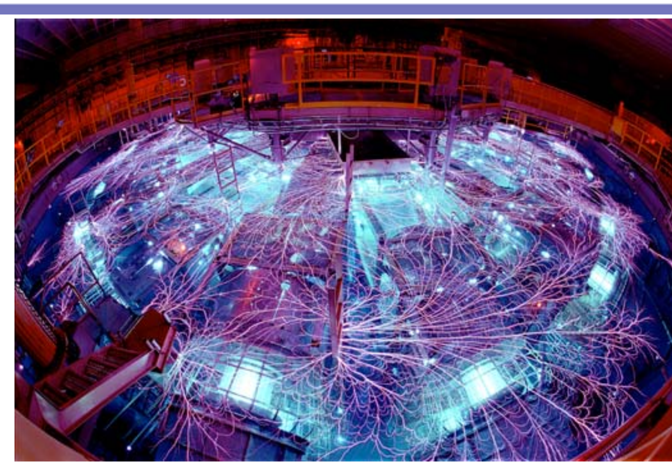


Courtesy of J. Richardson

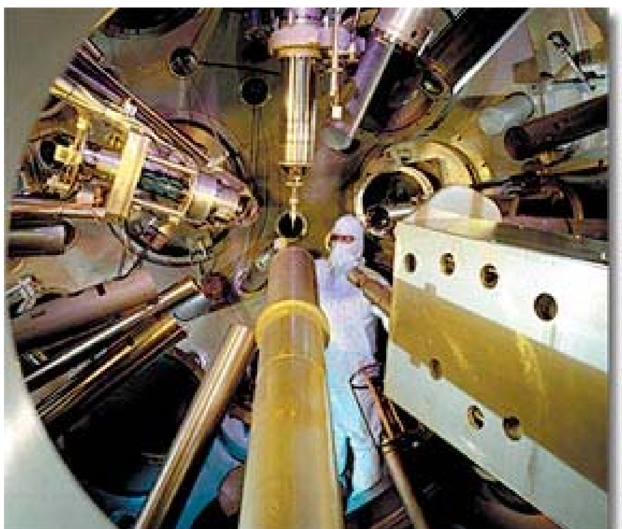
Current planetary models are consistent with mass-radius observations within error bars (except HD 209458b, which has a too large radius).

Study planetary interiors in the laboratory: shock wave experiments

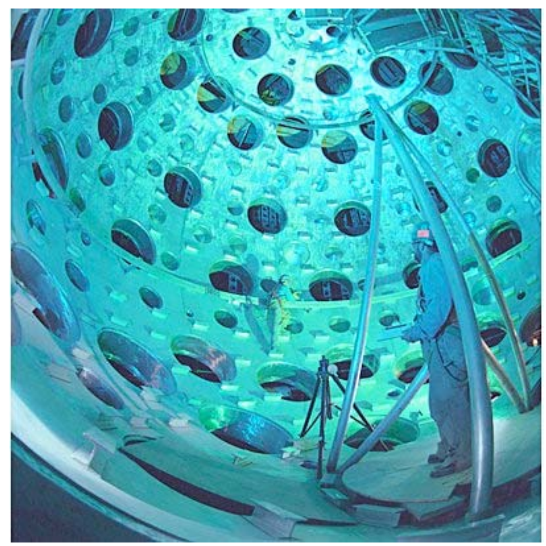
1) Two-stage gas gun (Livermore) 20 GPa



3) Z capacitor bank (Sandia) 175 GPa

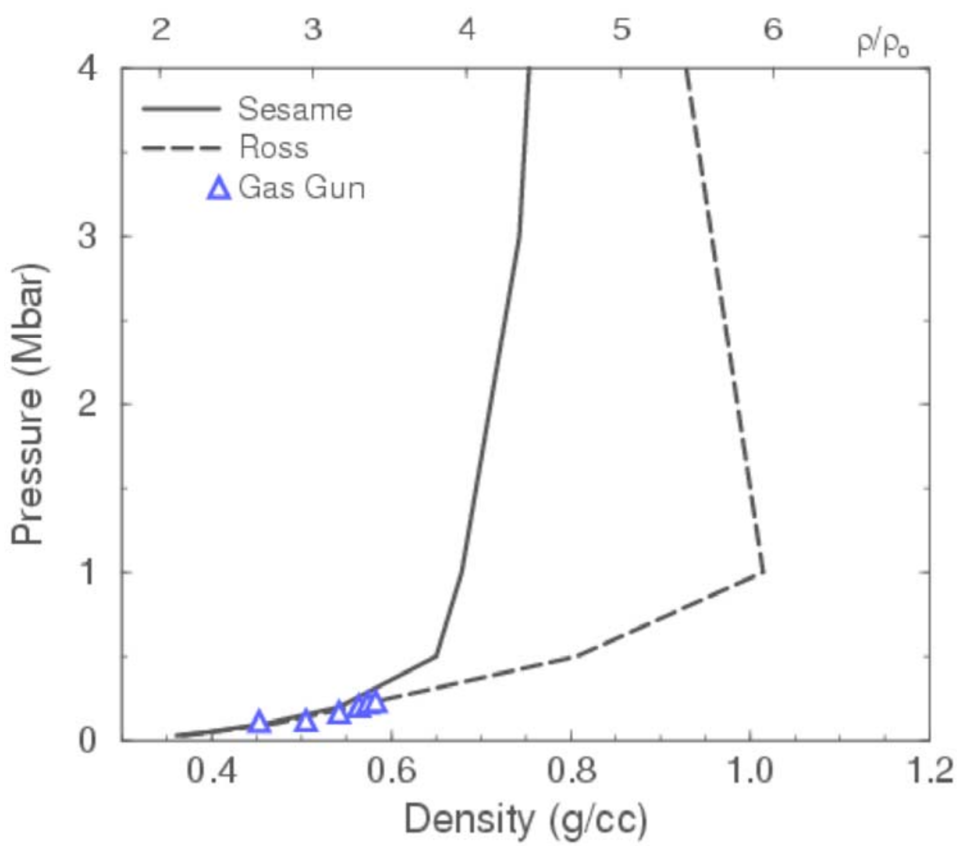


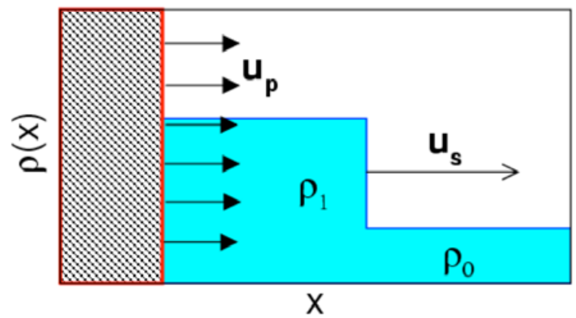
2) Nova laser (Livermore) 340 GPa



4) National Ignition Facility

Shock wave measurements determine the
EOS on the Hugoniot curve





Conservation of mass, momentum and energy yields:

$$\frac{\rho}{\rho_0} = \frac{u_s}{u_s - u_p}$$

$$p - p_0 = \rho_0 u_s u_p$$

$$E - E_0 = \frac{1}{2}(V_0 - V)(P + P_0)$$

Gas gun (LLNL), Sesame model (Kerley), linear mixing model (M.Ross)

Analogy of classical and quantum systems Introduction of density Matrix

Classical Boltzmann statistics:

$$Z_C = \sum_i e^{-\beta E_i}$$

Quantum systems: use the density matrix

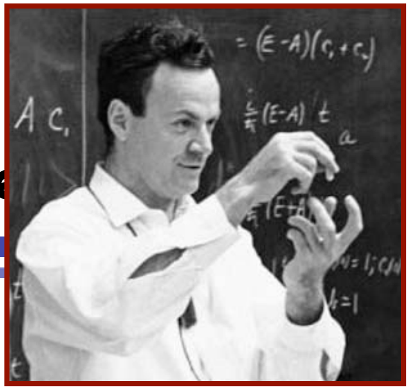
$$Z_C = Tr[\rho(R, R', \beta)]$$

$$\rho(R, R', \beta) = \sum_i \Psi_i(R) \; \Psi_i^*(R') \; e^{-\beta E_i}$$

$$\hat{\rho} = e^{-\beta \hat{H}}$$

Path Integrals in Imaginary Time

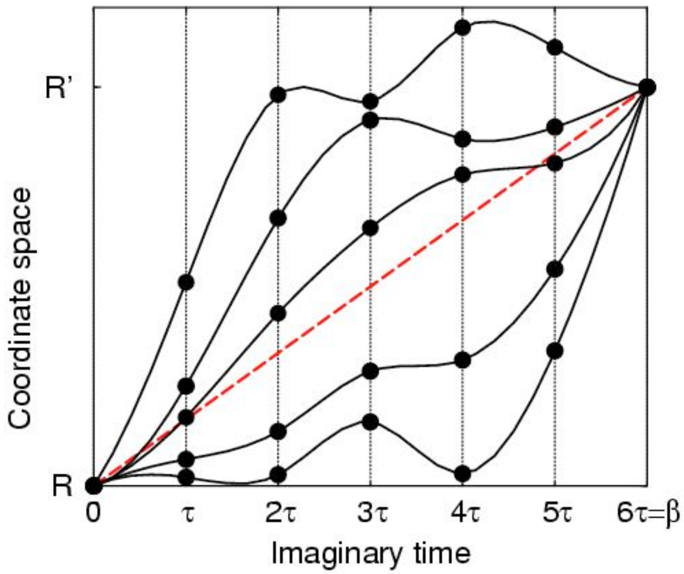
Every particle is represented by a path, a ring polyme



Density matrix: $$\hat{\rho} = e^{-\beta \hat{H}} = \left(e^{-\tau \hat{H}}\right)^M, \ \beta = \frac{1}{k_B T}, \ \tau = \frac{\beta}{M}$$

Trotter break-up:

$$\langle R | \hat{\rho} | R' \rangle = \langle R | (e^{-\tau \hat{H}})^M | R' \rangle = \int dR_1 \ldots \int dR_{M-1} \langle R | e^{-\tau \hat{H}} | R_1 \rangle \langle R_1 | e^{-\tau \hat{H}} | R_2 \rangle \ldots \langle R_{M-1} | e^{-\tau \hat{H}} | R' \rangle$$



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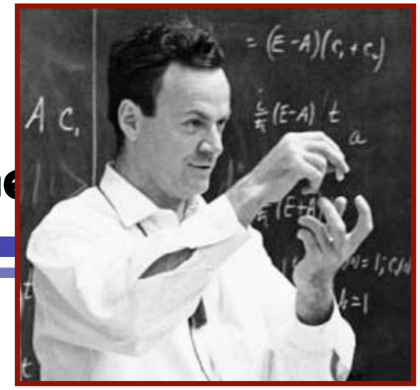


Density matrix:

$$\hat{\rho} = e^{-\beta\hat{\mathrm{H}}} = \left(e^{-\tau\hat{\mathrm{H}}}\right)^{M}, \quad \beta = \frac{1}{k_B T}, \quad \tau = \frac{\beta}{M}$$

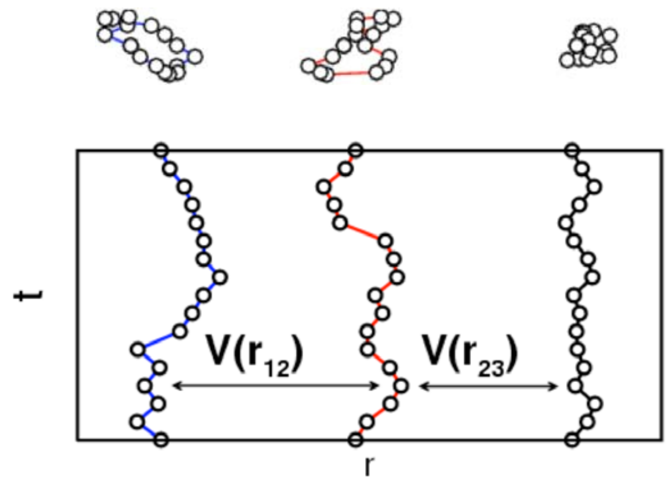
Trotter break-up:

$$\langle R | \hat{\rho} | R' \rangle = \langle R | (e^{-\tau\hat{\mathrm{H}}})^{M} | R' \rangle = \int dR_1 \ldots \int dR_{M-1} \langle R | e^{-\tau\hat{\mathrm{H}}} | R_1 \rangle \langle R_1 | e^{-\tau\hat{\mathrm{H}}} | R_2 \rangle \ldots \langle R_{M-1} | e^{-\tau\hat{\mathrm{H}}} | R' \rangle$$

Path integral and action:

$$\langle R | \hat{\rho} | R' \rangle = \oint_{R \to R'} dR_t e^{-S[R_t]}$$

$$S[R_t] = \sum_{i=1}^{M} \frac{(R_{i+1} - R_i)^2}{4\lambda\tau} + \frac{1}{2}[V(R_i) + V(R_{i+1})]$$



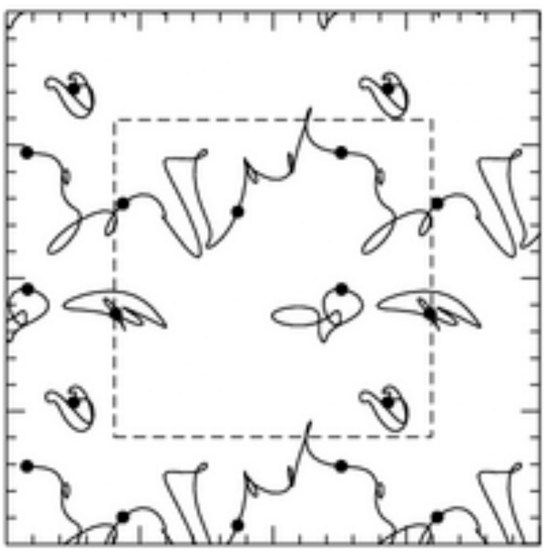
Start with solution of 2-particle problem → improved pair action

Particle Statistics: leads to exchange effects represented by permutations.

Symmetry leads to bosonic and fermionic path integrals

$$\langle R|\hat{\rho}_{F/B}|R'\rangle = \sum_P (\pm 1)^P \int dR_1 \ldots \int dR_{M-1} \langle R|e^{-\tau\hat{H}}|R_1\rangle \ldots \langle R_{M-1}|e^{-\tau\hat{H}}|PR'\rangle$$

Bosons: Long permutation cycles, only positive contributions → superfluidity in ^{4}He



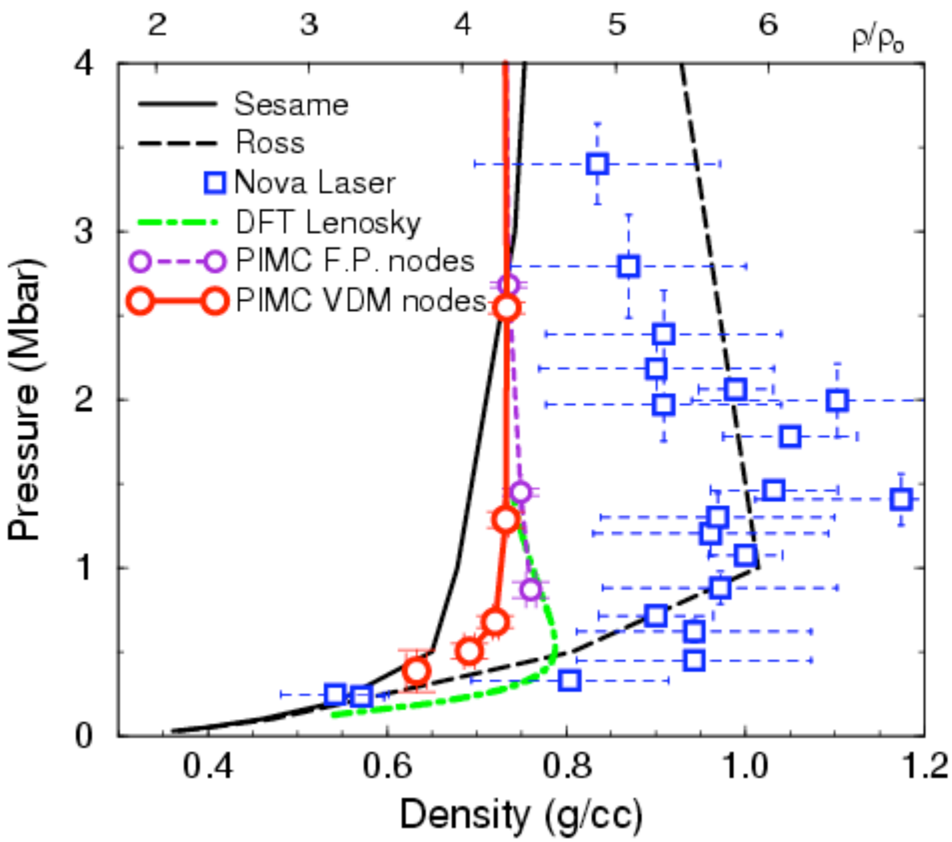
Fermions: Cancellation of positive and negative contributions → Fermion sign problem, efficiency $e^{-\beta N}$

Fixed node approximation

$$\langle R|\hat{\rho}_F|R'\rangle = \sum_P (-1)^P \oint_{\rho_T \geq 0} dR_t e^{-S[R_t]}$$

Deuterium Hugoniot

Path integral Monte Carlo results



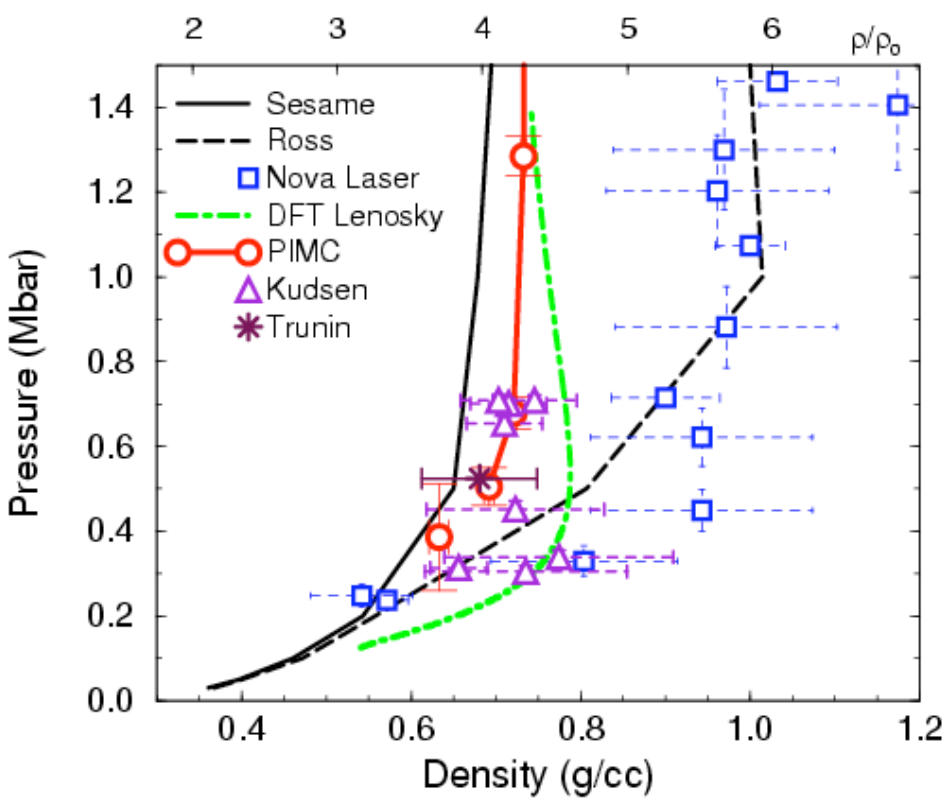
Militzer and Ceperley,
Phys. Rev. Lett. 85 (2000) 1890.
Phys. Rev. Lett. 87 (2001) 275502

- Accuracy increases with T
- Small size dependence
- Comparison of VDM and free particle nodes

Discrepancy:
$\Delta E/N = 3$ eV
$\Delta PV/N = -2$ eV

Good agreement between all *ab initio* methods.

PIMC predicts low compressibility and agrees with more recent experiments



Militzer, Ceperley *et al.*
Phys. Rev. Lett. **85** (2000) 1890.
Phys. Rev. Lett. **87** (2001) 275502.

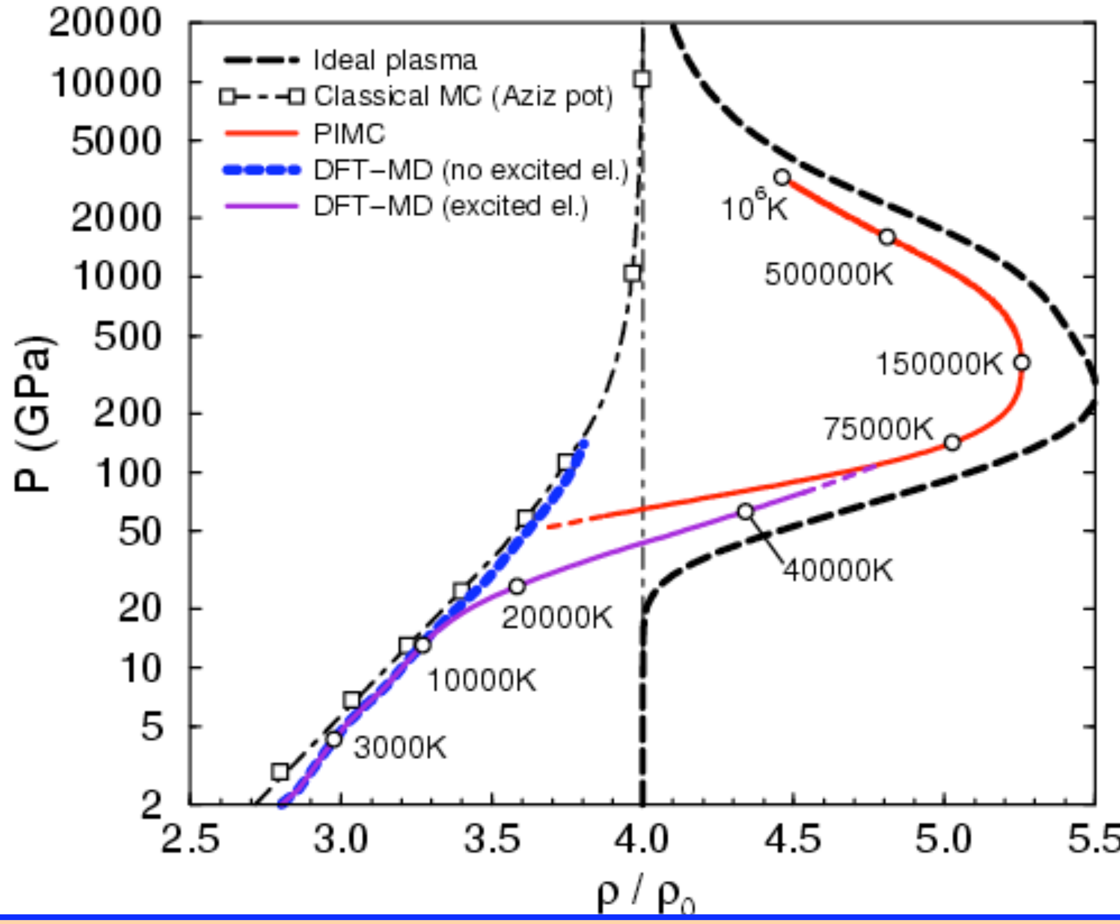
- Predict low compressibility!

Good agreement with:

- Magnetic shocks waves
  [Knudson *et al*., PRL **87** (2001) 225501]
- Spherical converging shock waves
  [Belov et al, Boriskov et al.]
- DFT results (e.g. Bonev et al.)

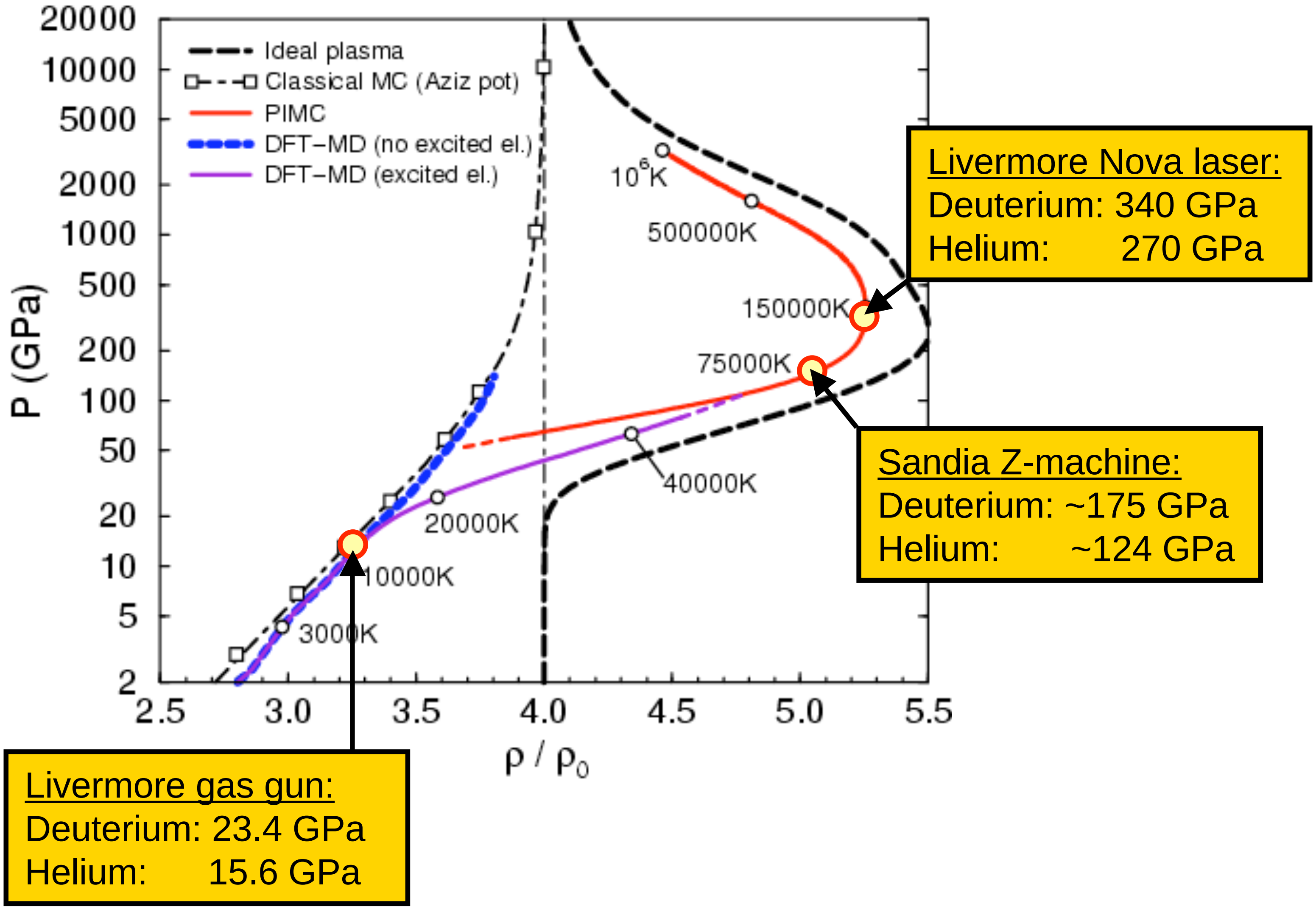
Recent measurements agree reasonably well with first principle methods but need to be verified.

PIMC results yield more than 5-fold compression [Militzer, Phys. Rev. Lett. 97 (2006) 175501]



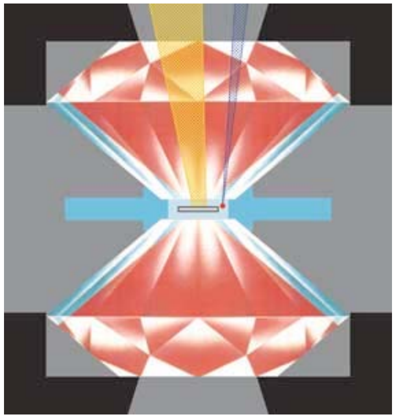
This high precompression is surprising because both PIMC and DFT-MD gave about 4-fold compression for hydrogen.

Laser and Z-machine can probe regime of 5-fold compression

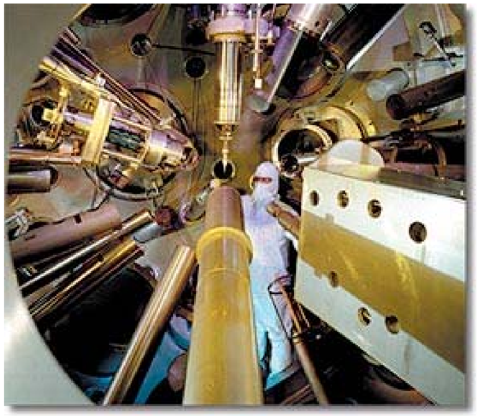


New Experimental Technique: Combination of Static and Dynamic Compression

1) Static compression
Diamond anvil cell

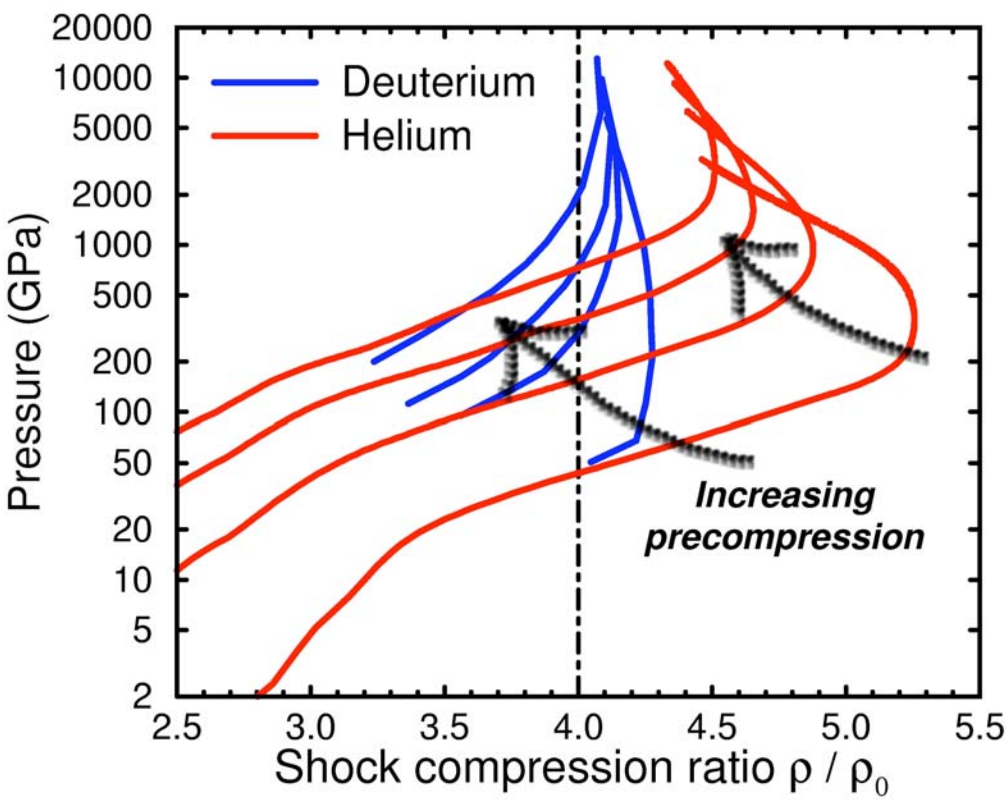


2) Dynamic shock comp.
Laser shocks



- Performed by laser shock group at LLNL in collaboration with P. Loubeyre (CEA)
- Samples are precompressed using a modified diamond anvil cell.
- Precompression up to 1.5 GPa = 15 kbar
- Mixtures of hydrogen and helium are studied.

Summary: Maximum shock compression in deuterium and helium



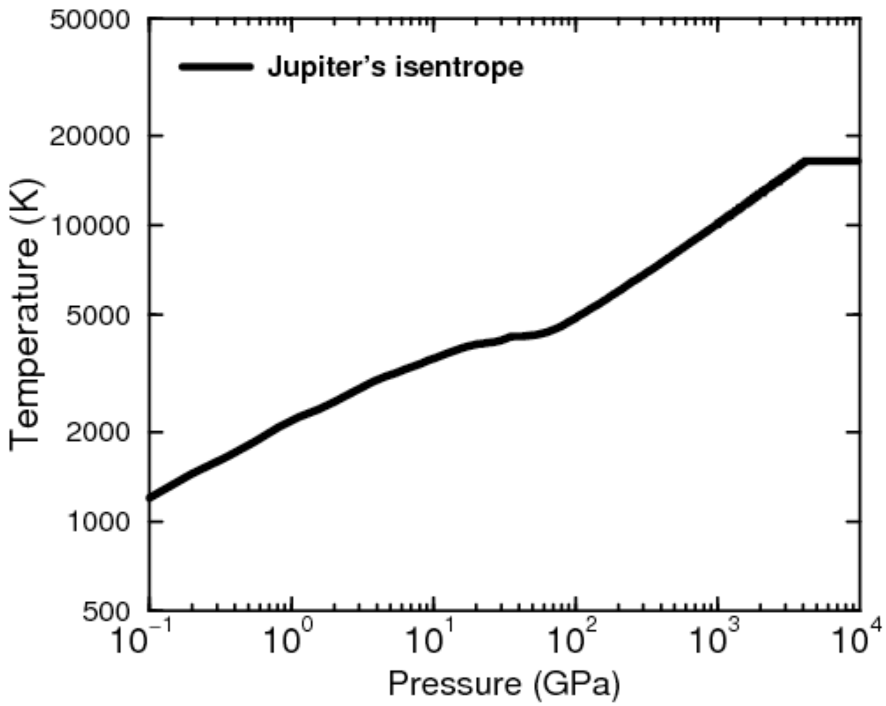
Maximum compression is controlled by

a) The excitation of internal degrees of freedom that increase the energy (higher compression)

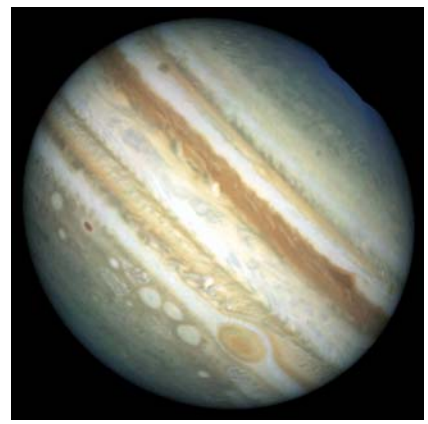
b) Interaction effects that increase the pressure (lower compression)

B. Militzer, "First-principles calculation of shock compressed fluid helium", *Physical Review Letters*, 97 (2006) 175501

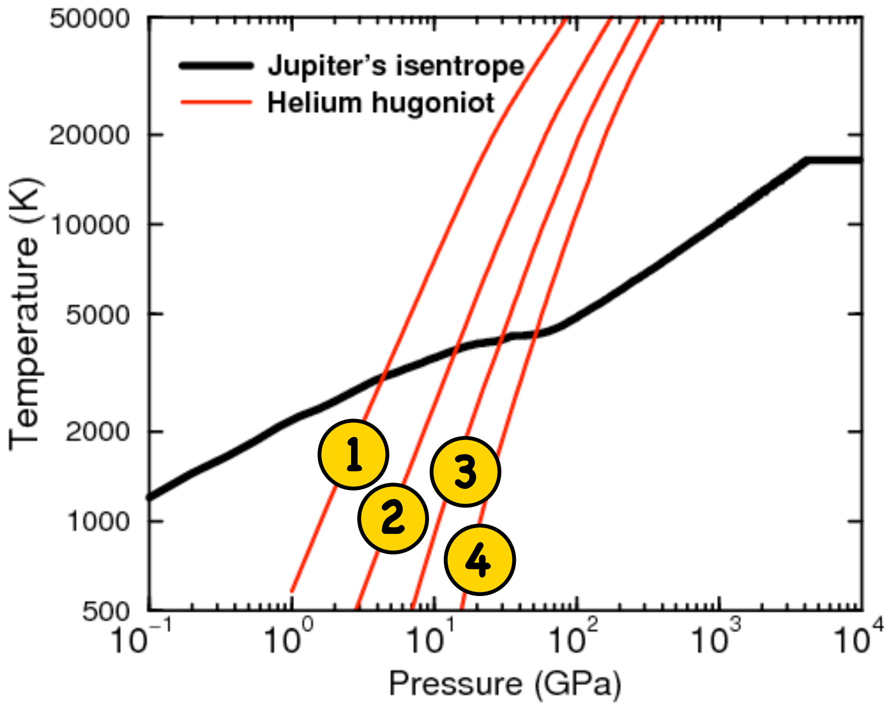
How far into in Jupiter's interior can be probe with precompressed shocks?



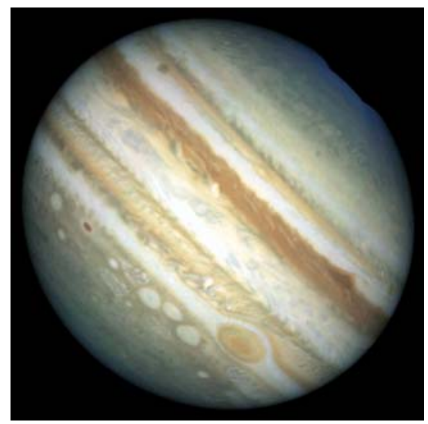
Where does the helium hugoniot intersect with Jupiter's isentrope?



How far into in Jupiter's interior can be probed with precompressed shocks?



Where does the helium hugoniot intersect with Jupiter's isentrope?



	Precompression	P_0	P_H(GPa)	T_H(K)	Mass fraction	$1-R_H/R_J$
He	1	1 bar	4.4	3000	0.5%	3%
He	2	188 bar	14	3750	1.6%	6%
He	3	1.8 kbar	29	4000	2.8%	8%
He	4	7.1 kbar	51	4200	4.6%	10%

Summary and Outlook

- **Observations:**
  1) Rapidly expanding set of known extrasolar planets
     ⇒ mass-radius relationship from transits
  2) Spectroscopic characterization of their atmosphere
- **Experiments:**
  1) expect new laser and magnetic compression results for He
  2) Combination of static and dynamic compression technique reach probe higher densities (back to shock reverberation?)
  3) Shocks with NIF
- **Theory:** EOS derived from first principles simulations, Answer questions about the structure and evolution of giant planets:
  1) Determine the properties of Jupiter's core?
  2) New models for extra solar giant planets.
  3) Mass-radius relationships for ice, water, and rocky planets.

Advertisements

- Summer school on "Quantum Monte Carlo: from Minerals and Materials to Molecules", Urbana, IL, July 9-19
- NSF Research Experience for Undergraduates program at Carnegie: Internships every summer

http://militzer.gl.ciw.edu