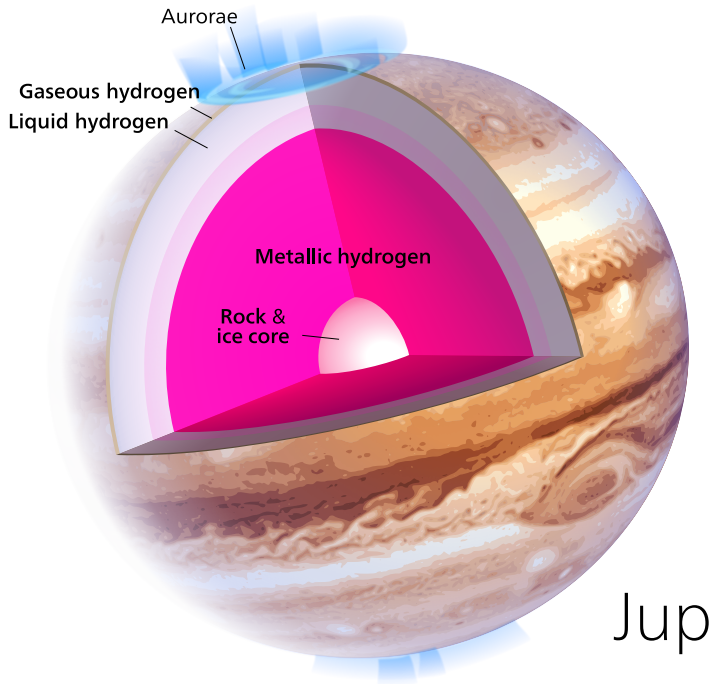
A unified modelization from condensed matter to plasmas

From the surface to the core of giant planets...



Jupiter

Augustin Blanchet

Gilles Maynard, Paris Sud, LPGP
Jean Clérouin, Marc Torrent
CEA, DAM, DIF, F-91297 Arpajon, France

www.cea.fr

Two kinds of computational methods

- $\mathbf{T} \lessapprox \mathbf{T_f}$: Kohn-Sham method
  - Wave functions are decomposed in a basis of plane waves:

$$\Psi_{\mathbf{k}}(\mathbf{r},\sigma) = \sum_{\mathbf{G}} u_{\mathbf{k}}(\mathbf{G},\sigma) e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$$

  - Very Accurate at low temperatures (molecular states).
  - Electronic properties (Kubo-Greenwood electrical conductivity).
  - At high temperature, we need to consider a lot of electronic orbitals.

Two kinds of computational methods

- $\mathbf{T} \lessapprox \mathbf{T_f}$: Kohn-Sham method
  - Wave functions are decomposed in a basis of plane waves:

$$\Psi_{\mathbf{k}}(\mathbf{r},\sigma) = \sum_{\mathbf{G}} u_{\mathbf{k}}(\mathbf{G},\sigma) e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$$

  - Very Accurate at low temperatures (molecular states).
  - Electronic properties (Kubo-Greenwood electrical conductivity).
  - At high temperature, we need to consider a lot of electronic orbitals.

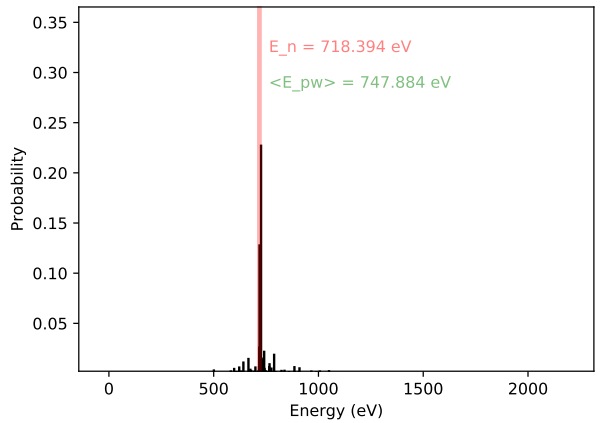
- $\mathbf{T} > \mathbf{T_f}$: Orbital free method
  - Same computing time regardless of the number of electrons.
  - Equivalent to consider wave functions as a unique plane wave, in a purely kinetic form.
  - Based on Thomas-Fermi methods that are inaccurate at low temperatures (no molecular states).
  - Kubo-Greenwood electrical conductivity isn't relevant.

Connexions to the free particle problem

- A lot of orbitals are needed to enforce a minimum filling.
- But high energy orbitals look like a single plane wave.
  It's a lot of work for nothing!
- Energies of states are getting closer from each other. $\Longrightarrow$
  We can consider a continuous regime past a certain energy which suggest to split contributions.

Number of orbitals to consider to ensure a minimal filling for a 64 Hydrogen box

Filling $\setminus \frac{T}{T_f}$	0	1	10	100
10^{-1}	32	87	207	586
10^{-3}	32	120	311	914
10^{-4}	32	133	350	1039
Comp. time	1"	1'12"	21'	9h30'



PW decomposition of a high energy orbital of $_{13}$Al in a FCC lattice

Splitting contributions in two parts

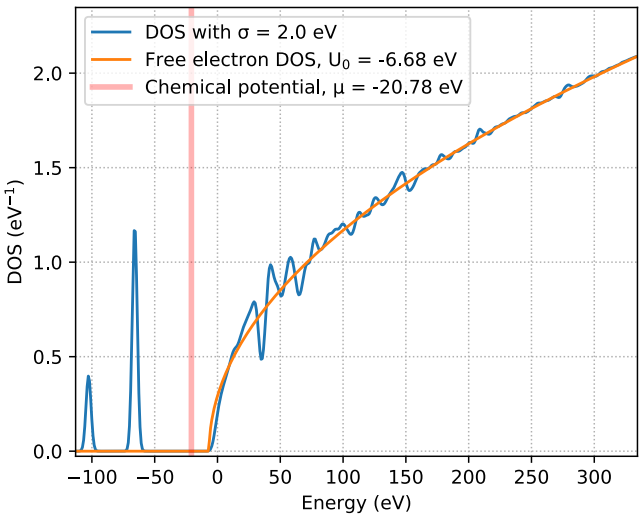
- The density of states tends to follow the free density of states.
- Contributions are splitted into descret sum and continuous sum [1].

- Electronic density contribution:

$$\rho(\mathbf{r}) = \sum_{i=1}^{N_c} f(\epsilon_i)|\Psi_i(\mathbf{r})|^2 + \frac{1}{\Omega}\int_{E_c}^{\infty} f(\epsilon) D(\epsilon) d\epsilon$$

$$D(\epsilon) = \frac{\sqrt{2}\Omega}{\pi^2}\sqrt{\epsilon - U_0}$$

Density of states of $_{13}$Al at 20 eV



Analog contributions are added to the expression of total energy, forces, pressure and stresses...

[1] Shen Zhang, Hongwei Wang, Wei Kang, Ping Zhang, and X. T. He. Physics of Plasmas, 23(4): 042707, April 2016.

Problematics to solve

- Physical problematics:
  - Introduction of an energy cut E_c for high temperature contribution.
  - The continuous limit is material dependant. Which criterion ?
  - Automatic choice of band cut to start high temperature procedure.

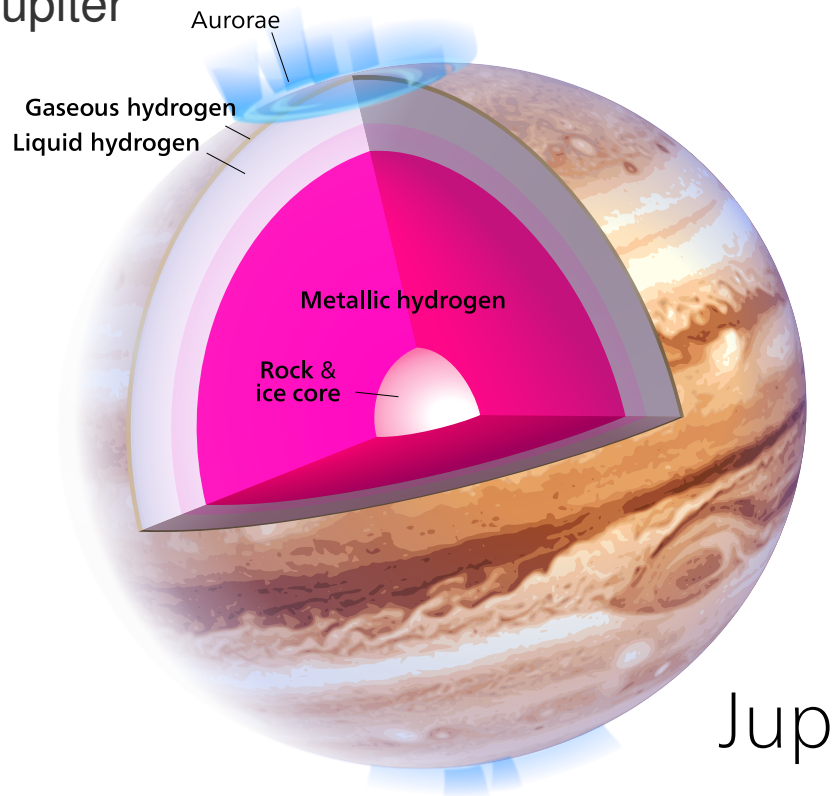
Problematics to solve

- Physical problematics:
  - Introduction of an energy cut E_c for high temperature contribution.
  - The continuous limit is material dependant. Which criterion ?
  - Automatic choice of band cut to start high temperature procedure.

- What should be done in the code:
  - Adding a continous contribtion to physical quantities to:
    Electronic density (`m_mkrho` $\rightarrow$ `mkrho`)
    Total energy (`m_scfcv_core` $\rightarrow$ `etotfor`)
    Stresses (`m_stress` $\rightarrow$ `stress`)
    Forces (`m_scfcv_core` $\rightarrow$ `etotfor`)
  - Adapt these contributions to the PAW formalism.
  - Explicitely express high temperature wave functions with reduced number of plane waves (`m_scfcv_core` $\rightarrow$ `scfcv_core`).
  - Adapt the Kubo-Greenwood electrical conductivity expression.
  - Automatic choice between standard or high temperature procedure.

Verifying the model and Possible applications

- To test the algorithm
  - Compare to orbital free model for high temperature systems
  - Make an hugoniot of Hydrogen with this algorithm
  - Follow an isentrope of Jupiter



Jupiter

[2] Jupiter diagram (modified): wikipedia.org/wiki/File:Jupiter_diagram.svg