MOLECULAR DYNAMICS AND EQUATIONS OF STATE FOR PLANETARY MODELING

JOURNÉE DES DOCTORANTS DU LUTH
3 JUILLET 2014

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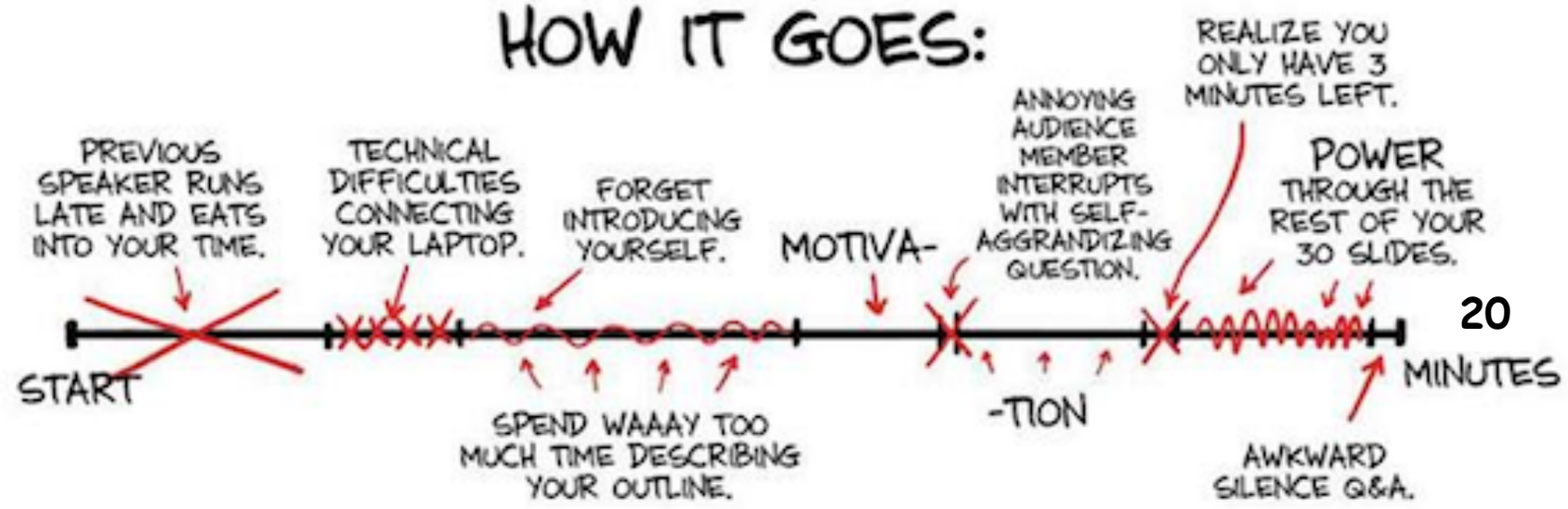
HOW I PLANNED IT:

HOW IT GOES:



OUTLINE

- **Exoplanet Quest**
- **Planetary Models**

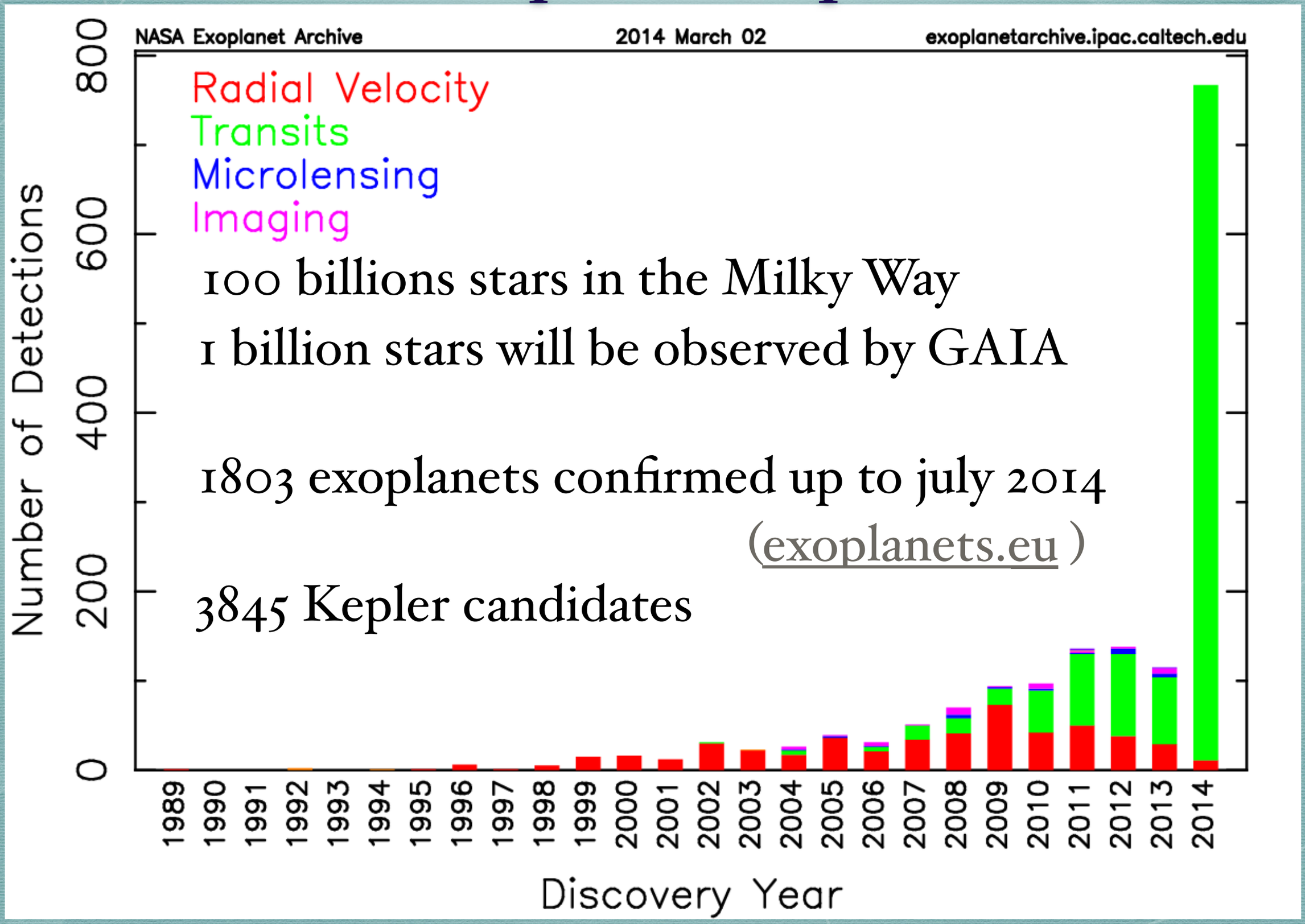
} Motivations

- **Numerical Simulations**
- **Equations of state**

} Methods

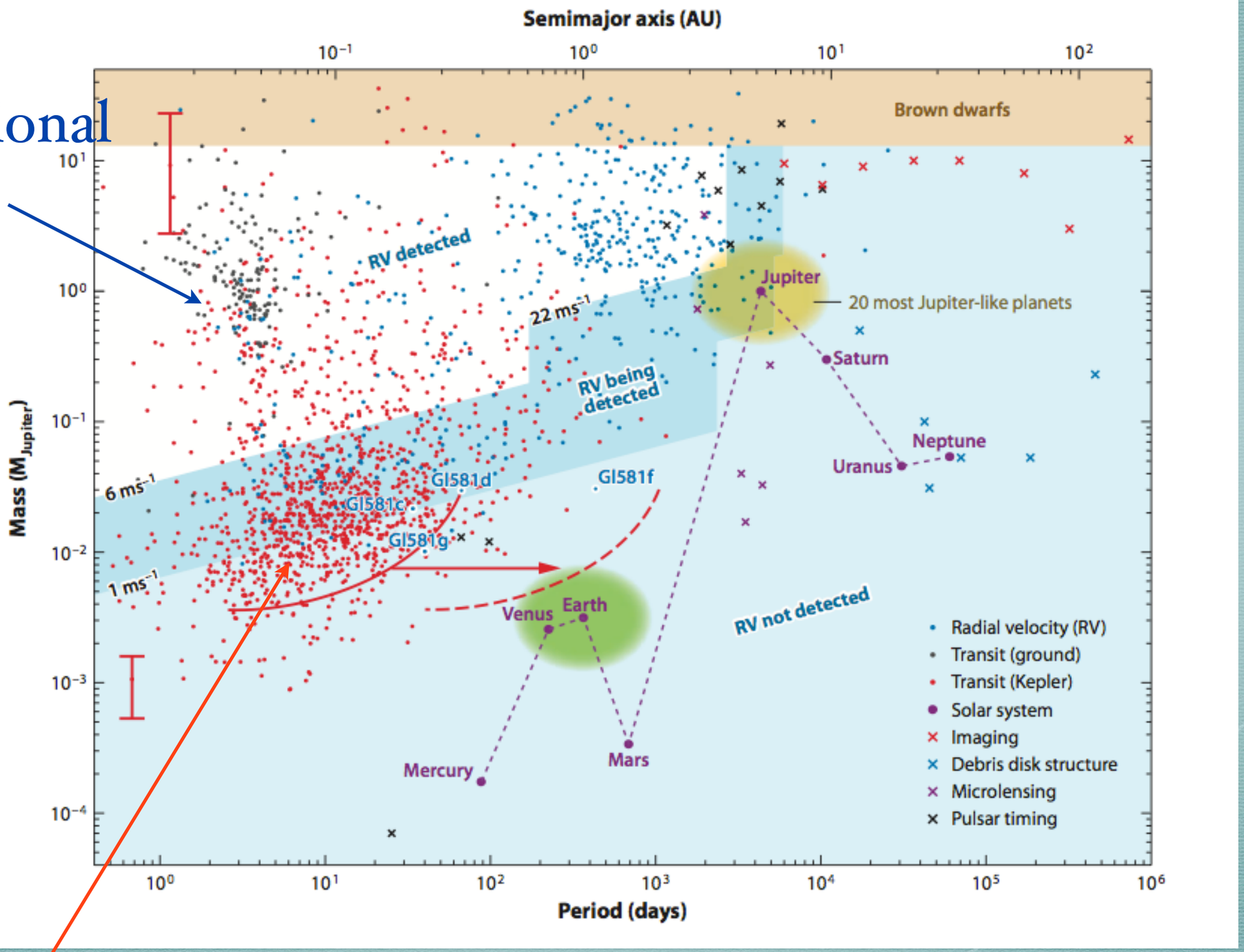
- **Results, Conclusions and Perspectives**

Exoplanets quest



Exoplanets quest

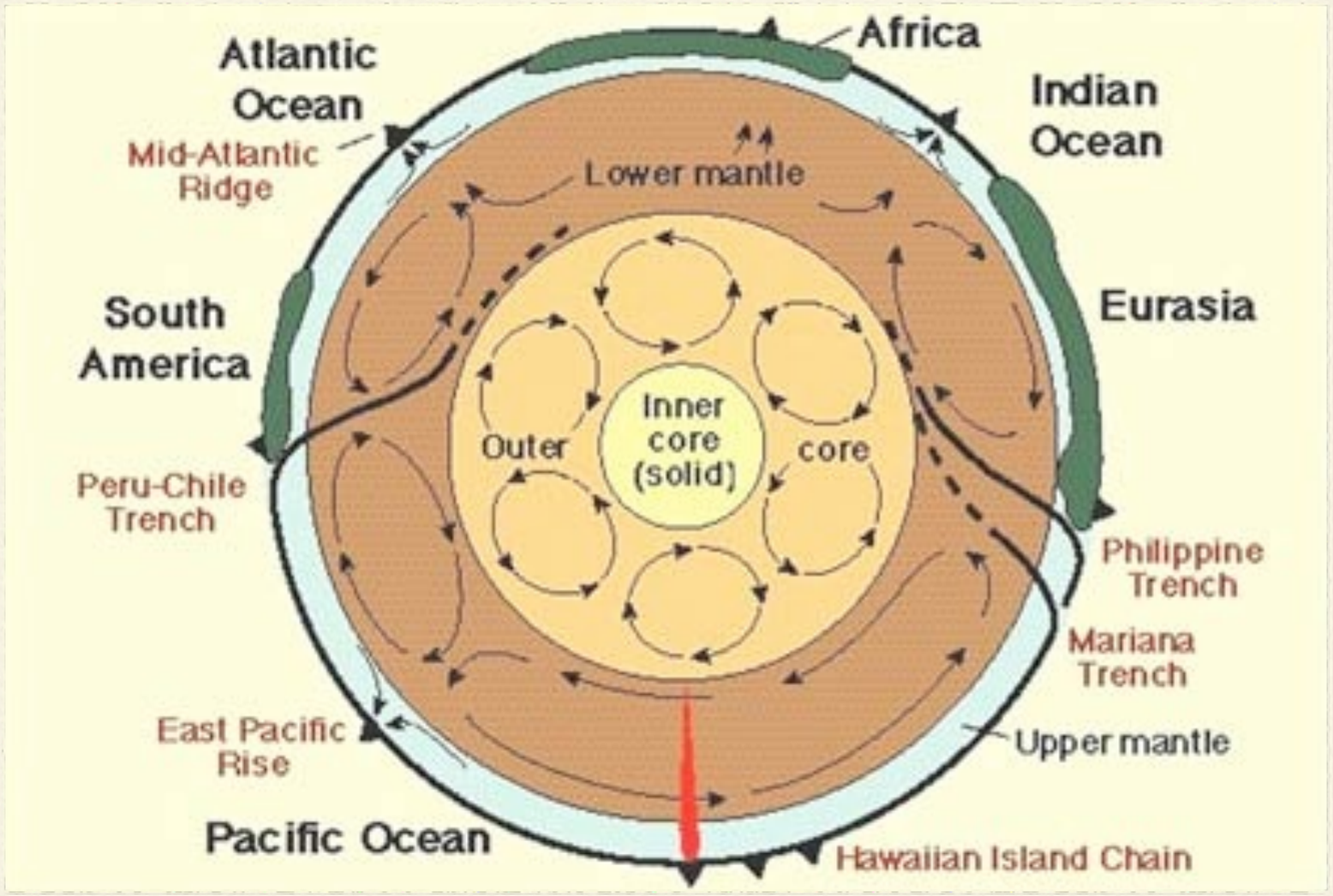
observational bias



about one hundreds super Earths

Terrestrial model

Earth stucture



Planetary equations

$$dP = -\rho g dr$$

$$m(r) = 4\pi \int_0^r r^2 \rho(r) dr$$

$$\frac{dT}{dr} = \frac{g\gamma}{\Phi} T$$

$$K = -V \frac{dP}{dV}$$

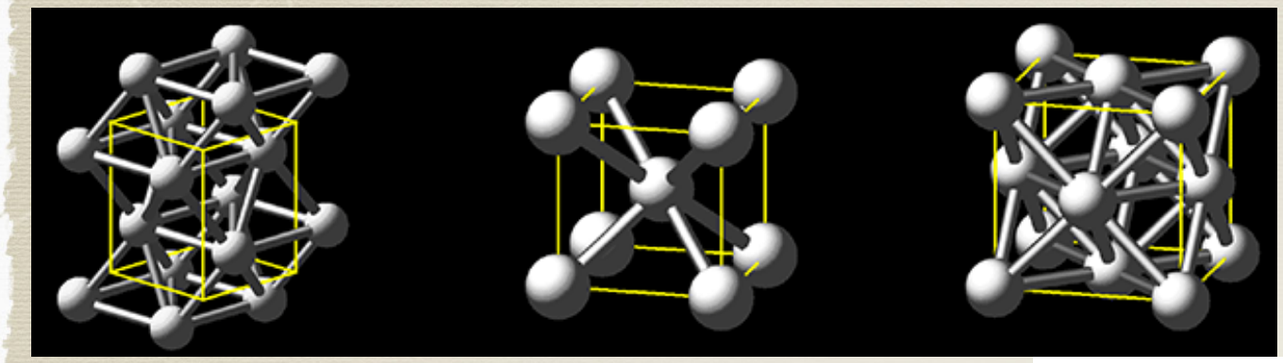
O, Mg, Si, Fe alone together represent the 95% of Earth mass!
(and in general of a rocky core: of Jupiter for example)

PlanetLab project

Simulations and experiments to inquire the most abundant elements and compounds, notably:

- Fe
- Fe alloys (Fe-Si, Fe-O, ...)
- SiO_2 (quartz for exemple)
- $MgSiO_3$ (perovskites, post-perovskite)

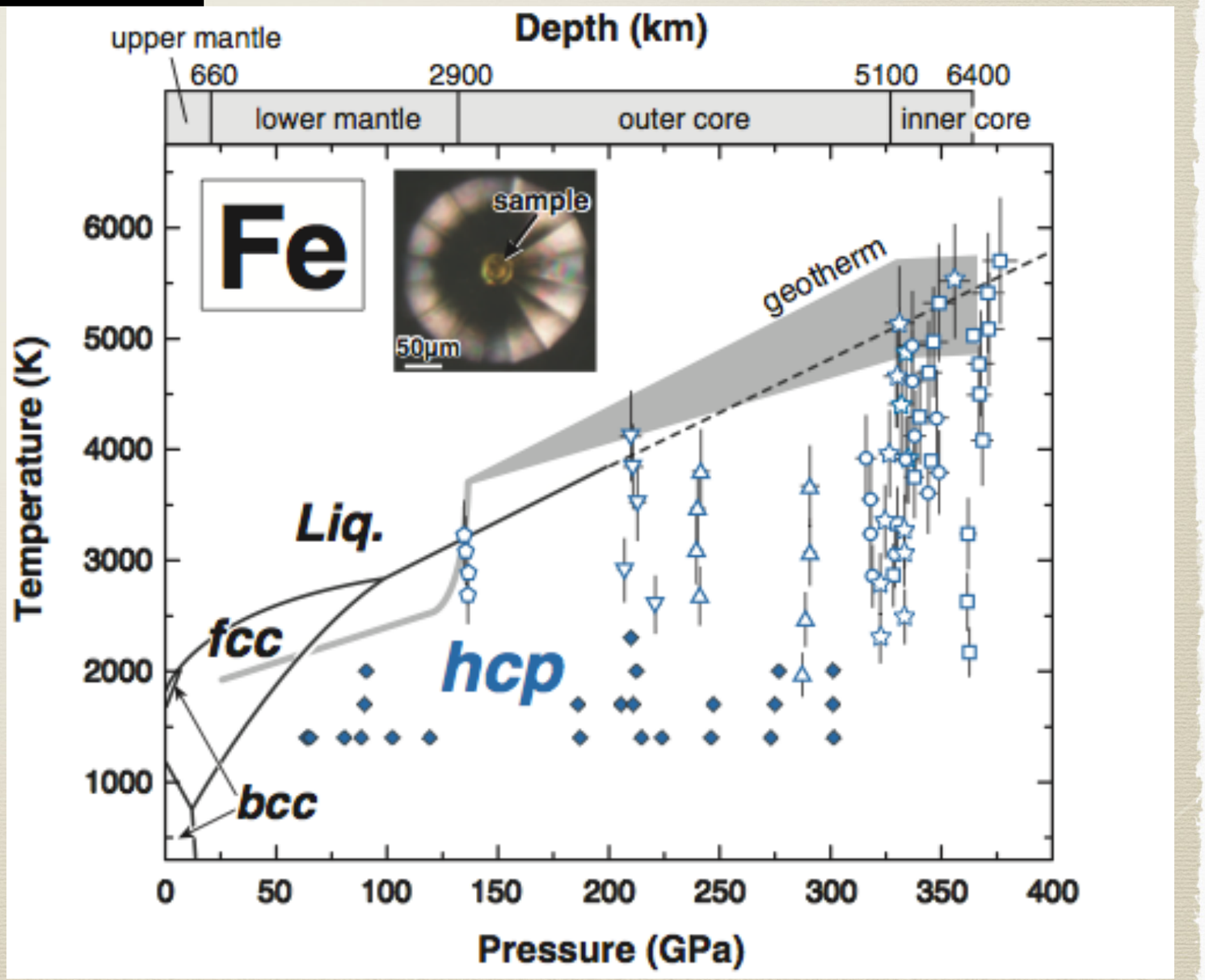
The example of iron



- hcp (hexagonal close-packed)
- bcc (body centered cubic)
- fcc (face centered cubic)

Three ways to investigate a phase diagram:

- Laser shock compression
- Heated diamond anvil cell
- Numerical simulations

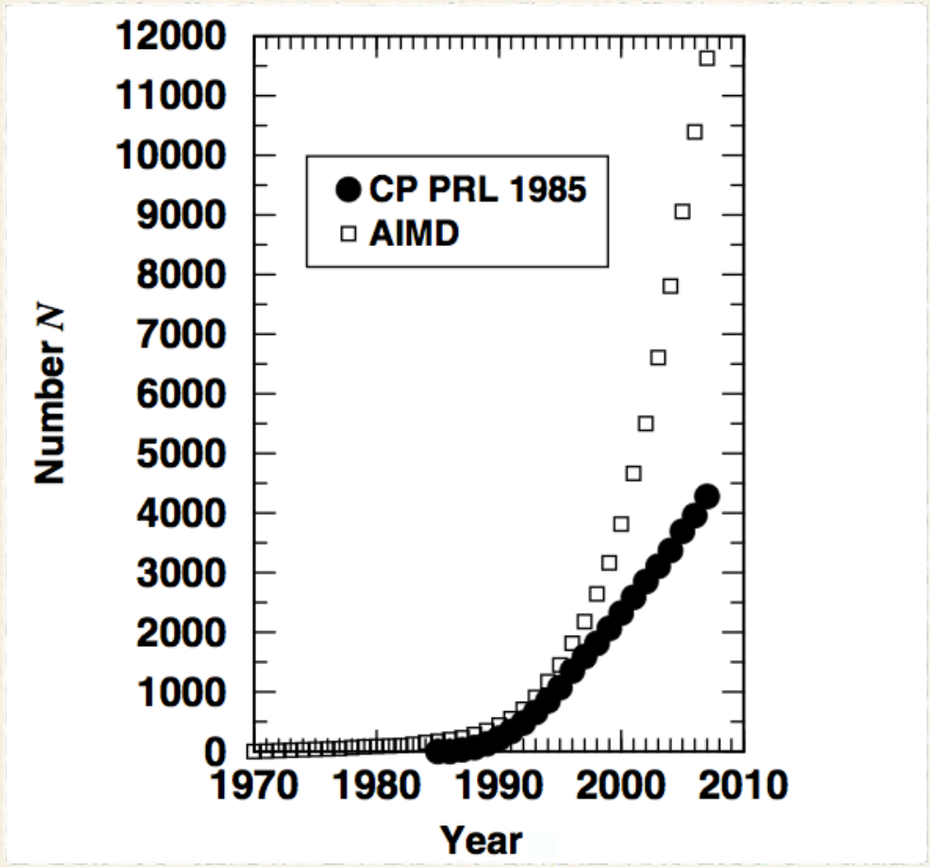


Molecular dynamics simulations

Ab Initio Molecular Dynamics (AIMD)

Widely employed in:

- chemistry
- molecular biology
- physics



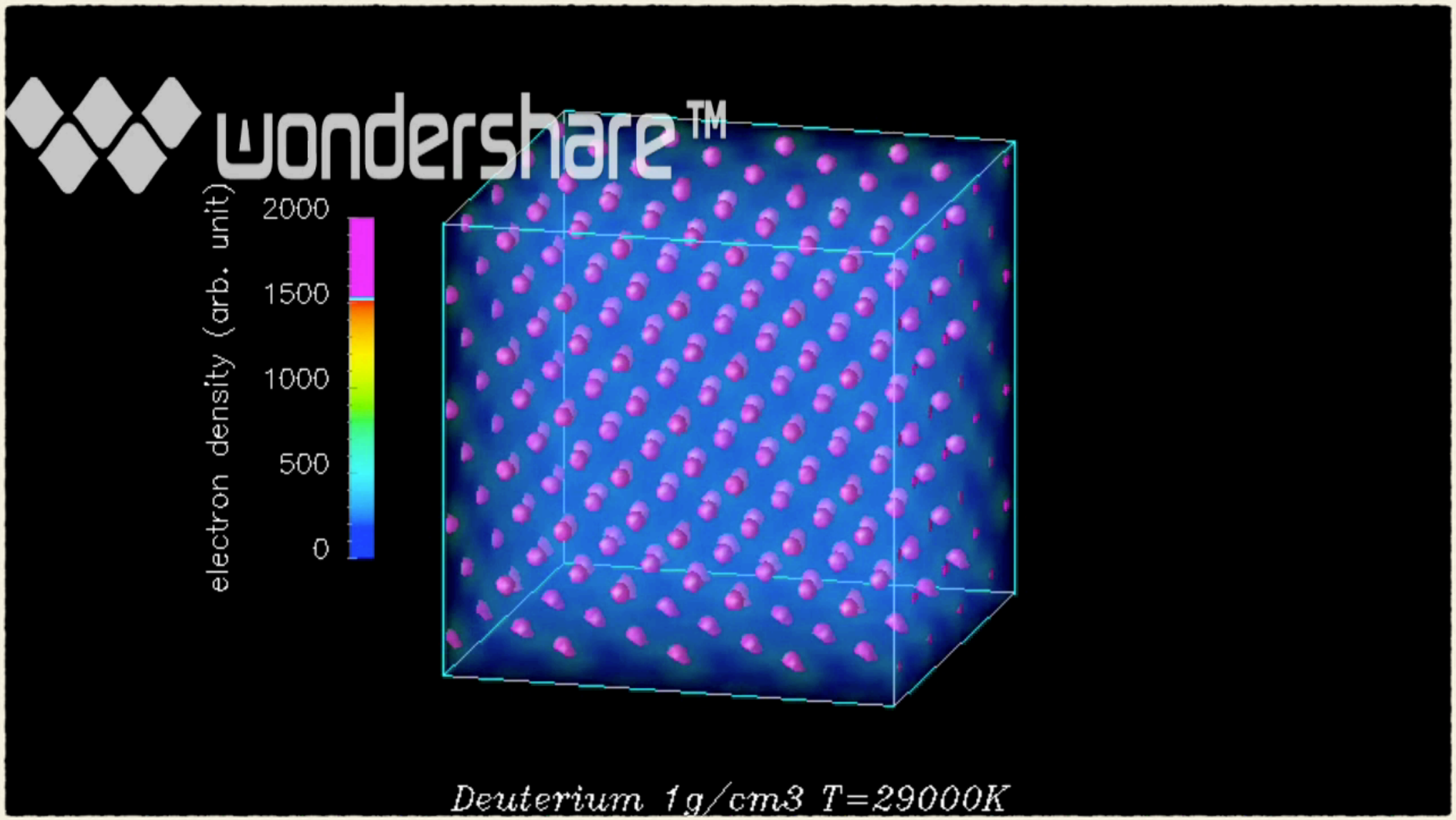
MICROSCOPICAL APPROACH:

N BODY PROBLEM OF INTERACTING NUCLEI AND ELECTRONS

$$H = \sum_{k=1}^{N_i} \frac{p_k^2}{2M_k} + \sum_{k=1}^{N_i} \sum_{k'<k} \frac{Z_k Z_{k'} e^2}{|\mathbf{R}_k - \mathbf{R}_{k'}|} + \sum_{l=1}^{N_e} \frac{p_l^2}{2m_l} + \sum_{l=1}^{N_e} \sum_{l'<l} \frac{e^2}{|\mathbf{r}_l - \mathbf{r}_{l'}|} + \sum_{k=1}^{N_i} \sum_{l=1}^{N_e} \frac{Z_k e^2}{|\mathbf{R}_k - \mathbf{r}_l|}$$

NOBODY CAN SOLVE IT EXACTLY!

Little visual exemple:



$$H = \sum_{k=1}^{N_i} \frac{p_k^2}{2M_k} + \sum_{k=1}^{N_i} \sum_{k'<k} \frac{Z_k Z_{k'} e^2}{|\mathbf{R}_k - \mathbf{R}_{k'}|} + \sum_{l=1}^{N_e} \frac{p_l^2}{2m_l} + \sum_{l=1}^{N_e} \sum_{l'<l} \frac{e^2}{|\mathbf{r}_l - \mathbf{r}_{l'}|} + \sum_{k=1}^{N_i} \sum_{l=1}^{N_e} \frac{Z_k e^2}{|\mathbf{R}_k - \mathbf{r}_l|}$$

Numerical simulations

- SOFTWARE ABINIT

Pseudopotential
Density Functional Theory
Plane wave basis

INPUT:

- Temperature
- Density (lattice parameter)
- Crystal structure
- How many plane wave (E_{cut})
- Number of valence electrons (Pseudopotential)
- Time step
- Number of atoms
- Convergence criteria

OUTPUT:

- Total energy
- Eigenvalues
- Eigenstates
- Density of states
- Stress tensor components
- Forces
- Nucleus trajectories

Numerical simulations

MEANS OF CALCULATION

Supercomputer like Titane at Centre de Calcul Recherche et Technologie

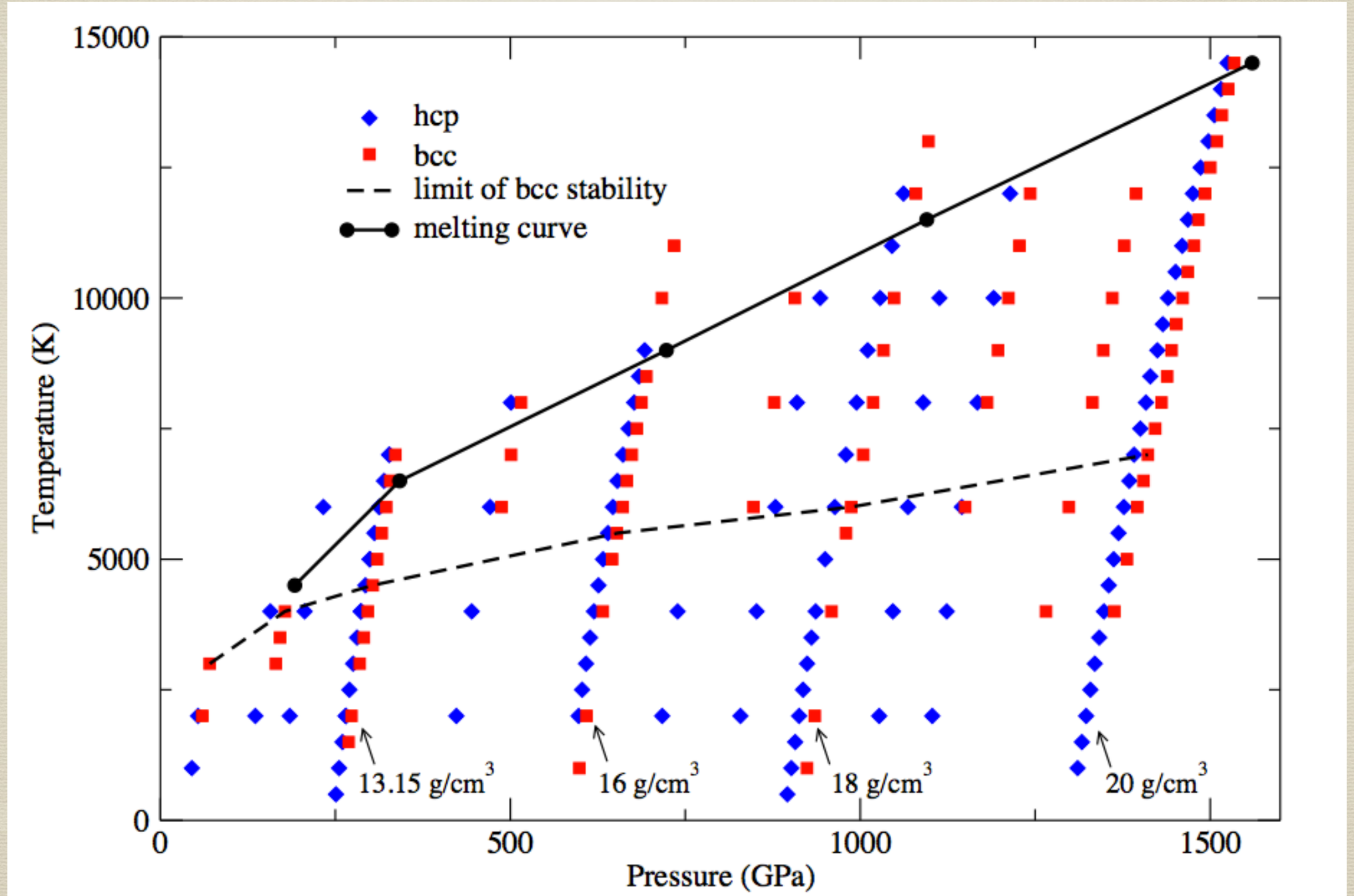
200-300 processors quad-core Intel Xeon 5570
for a total power of 300 Tflops

Every simulation took about 24 hours

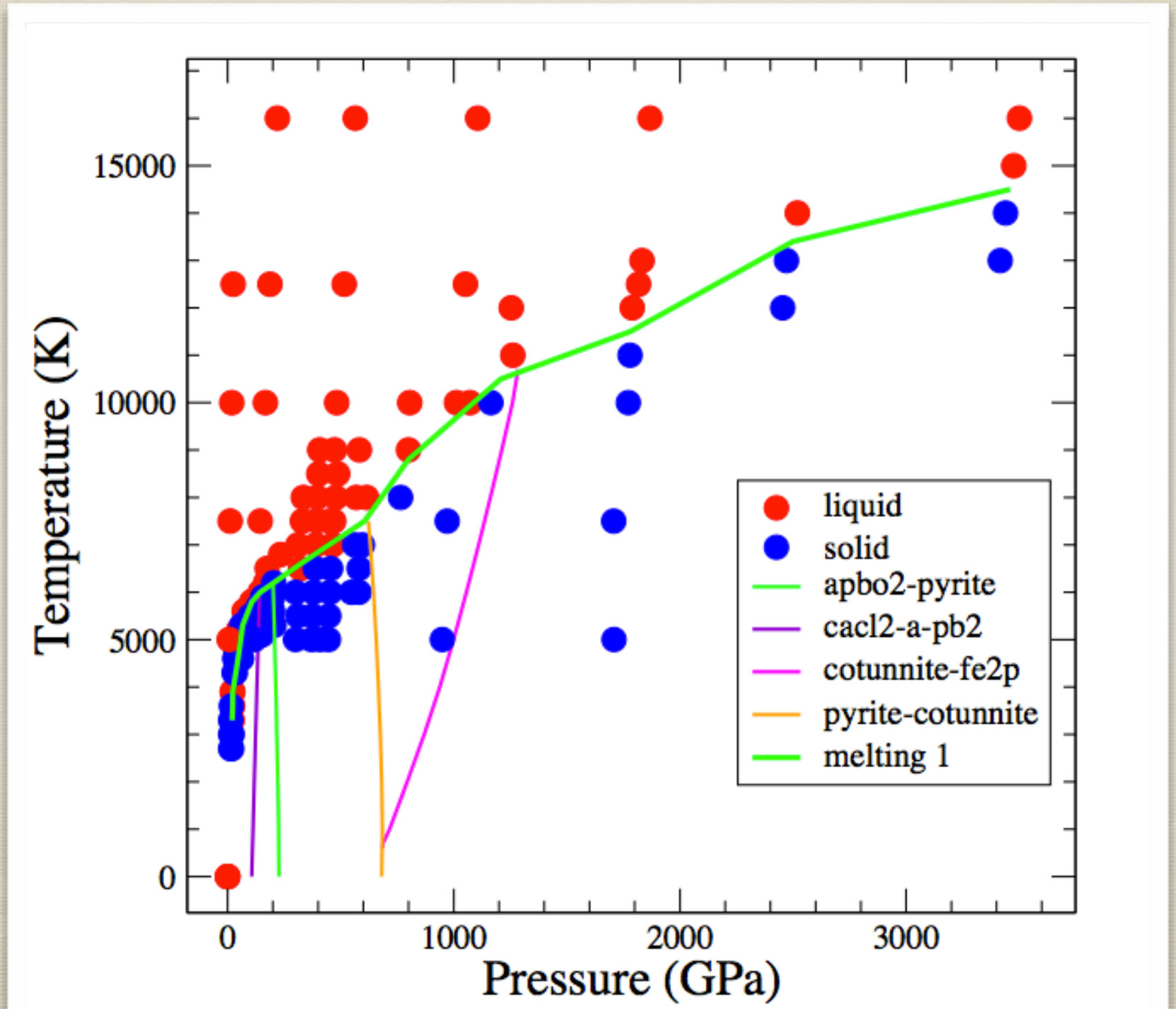
~200 runs

~5000 hours of total computation

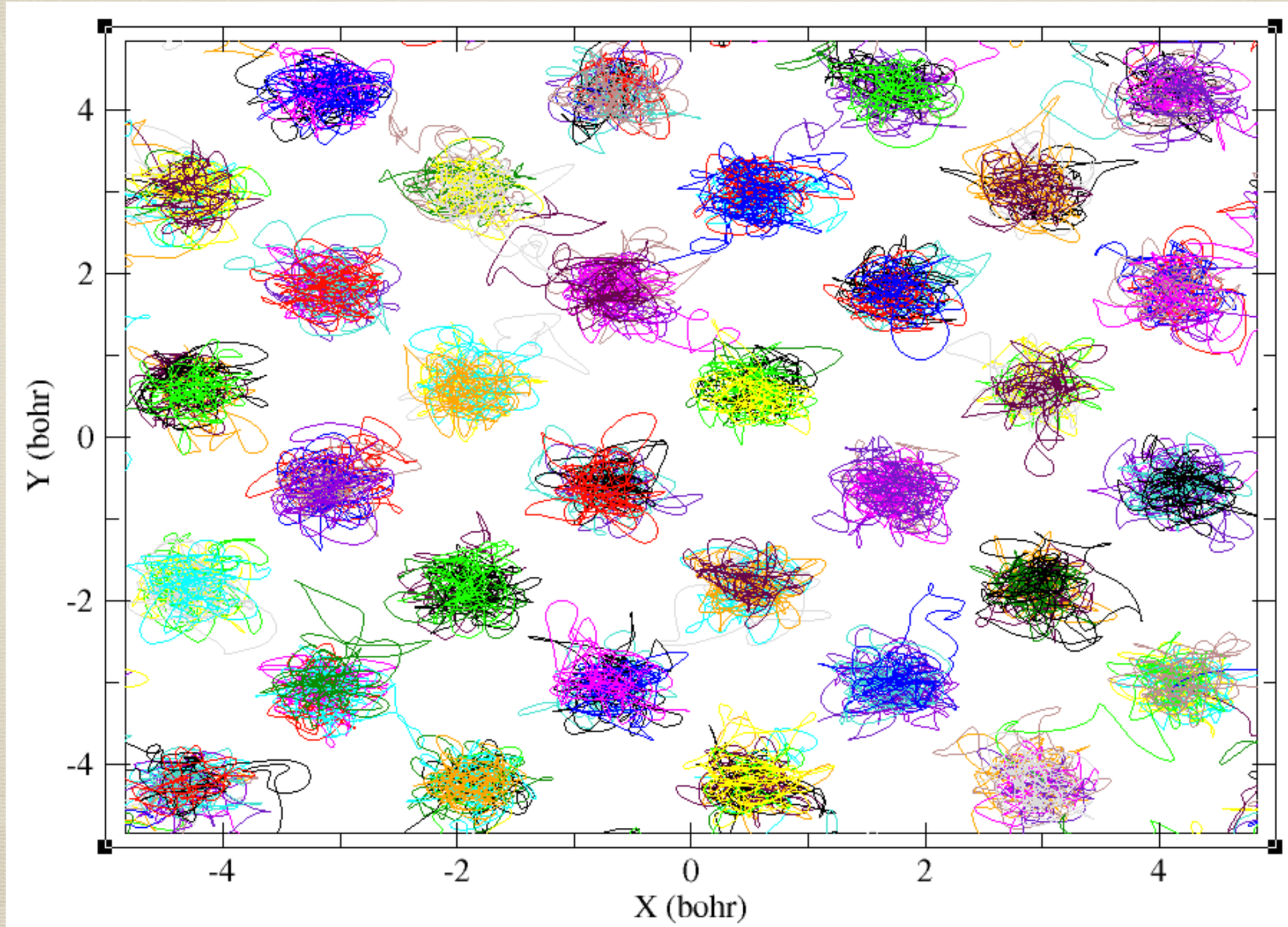
Overview of iron results



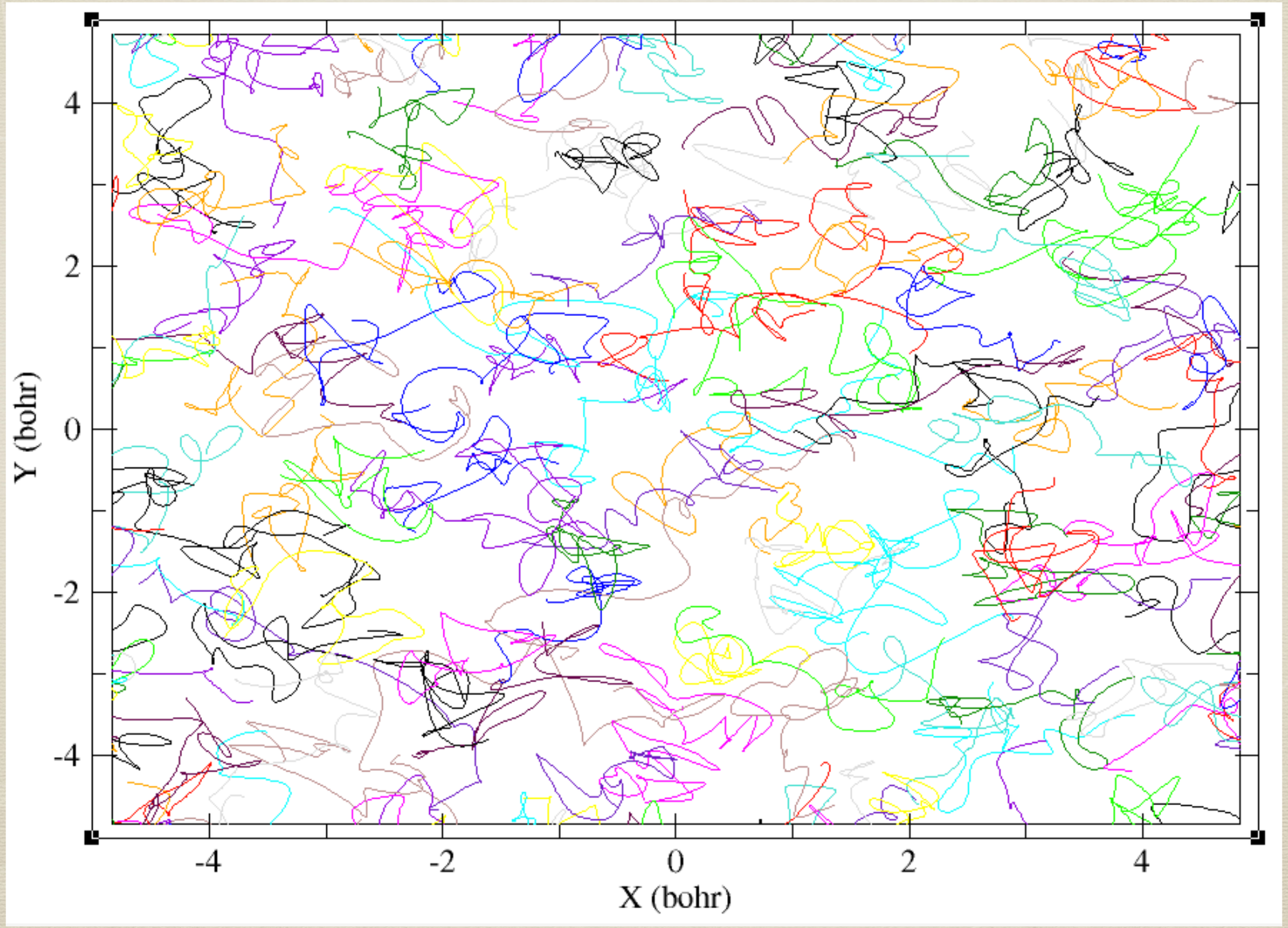
ABINIT data and melting curve for quartz



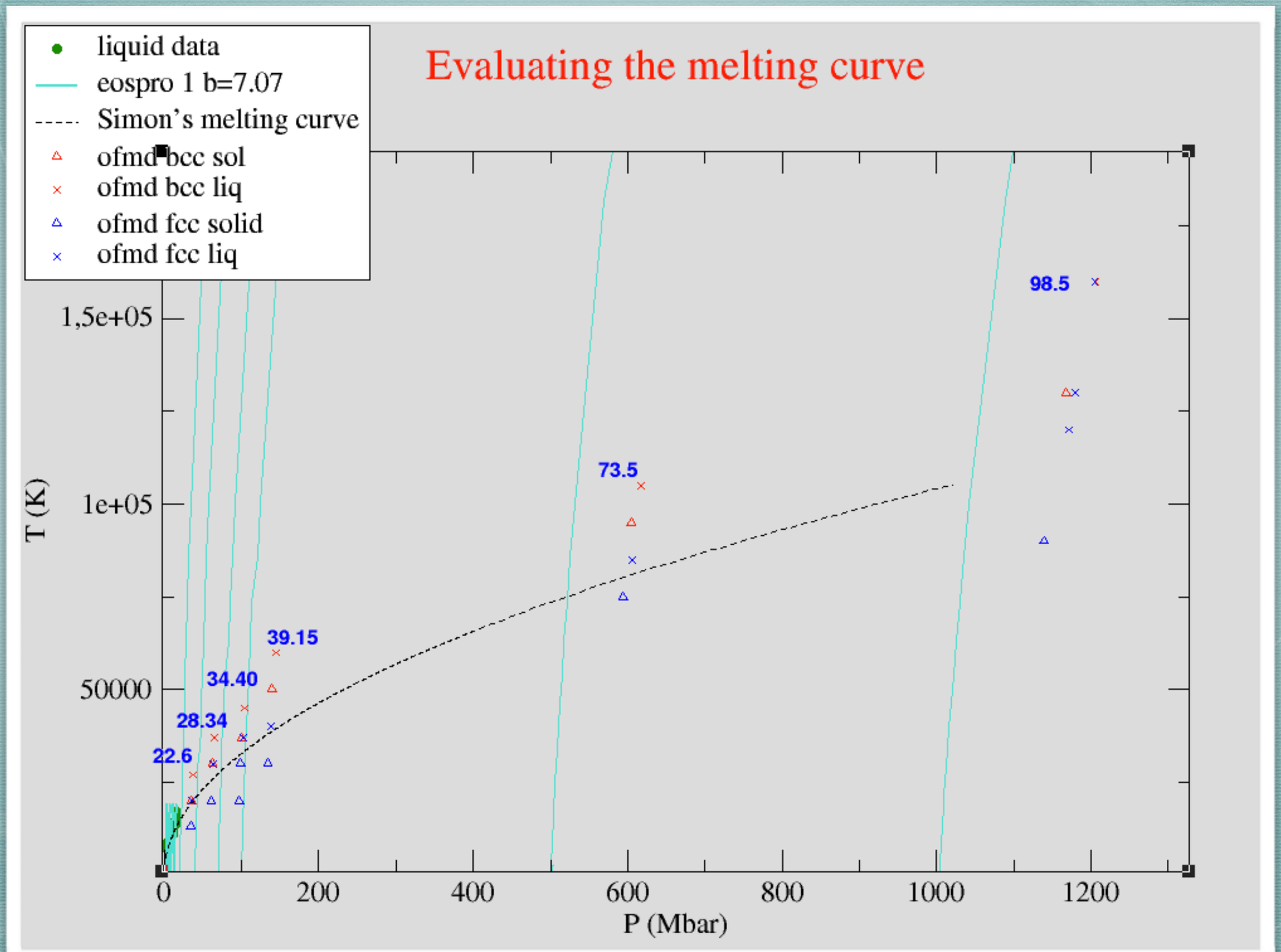
Heat Until it Melts (HUM)



Heat Until it Melts (HUM)



Melting curve up to 100 Mbar for iron



Fit of PVT solid data

Holzapfel EoS for the cold part:

$$P(V) = 3K_0 X^5 (1-X) \exp[c_0(1-X)][1 + c_2 X(1-X)$$

$X = (V/V_0)$

$c_0 = -\ln(3K_0/PFG_0)$

$c_2 = 3/2(K-3) - c_0$

$PFG_0 = 1003.6(Z/V_0)^{5/3}$

Einstein model for the thermal part:

$$P_{harm} = \gamma \frac{E_{harm}}{V}$$

$$E_{harm} = 3nR\left[\frac{\Theta}{2} + \frac{\Theta}{\exp(\Theta/T) - 1}\right]$$

$$\gamma = \gamma_\infty + (\gamma_0 - \gamma_\infty)(V/V_0)^\beta$$

$$\Theta = \Theta_0 (V/V_0)^{-\gamma_\infty} \exp\left[\frac{\gamma_0 - \gamma_\infty}{\beta}(1 - (V/V_0)^\beta)\right]$$

Anharmonic contribution:

$$P_a = \frac{3R}{2V} m a_0 X^m T^2$$

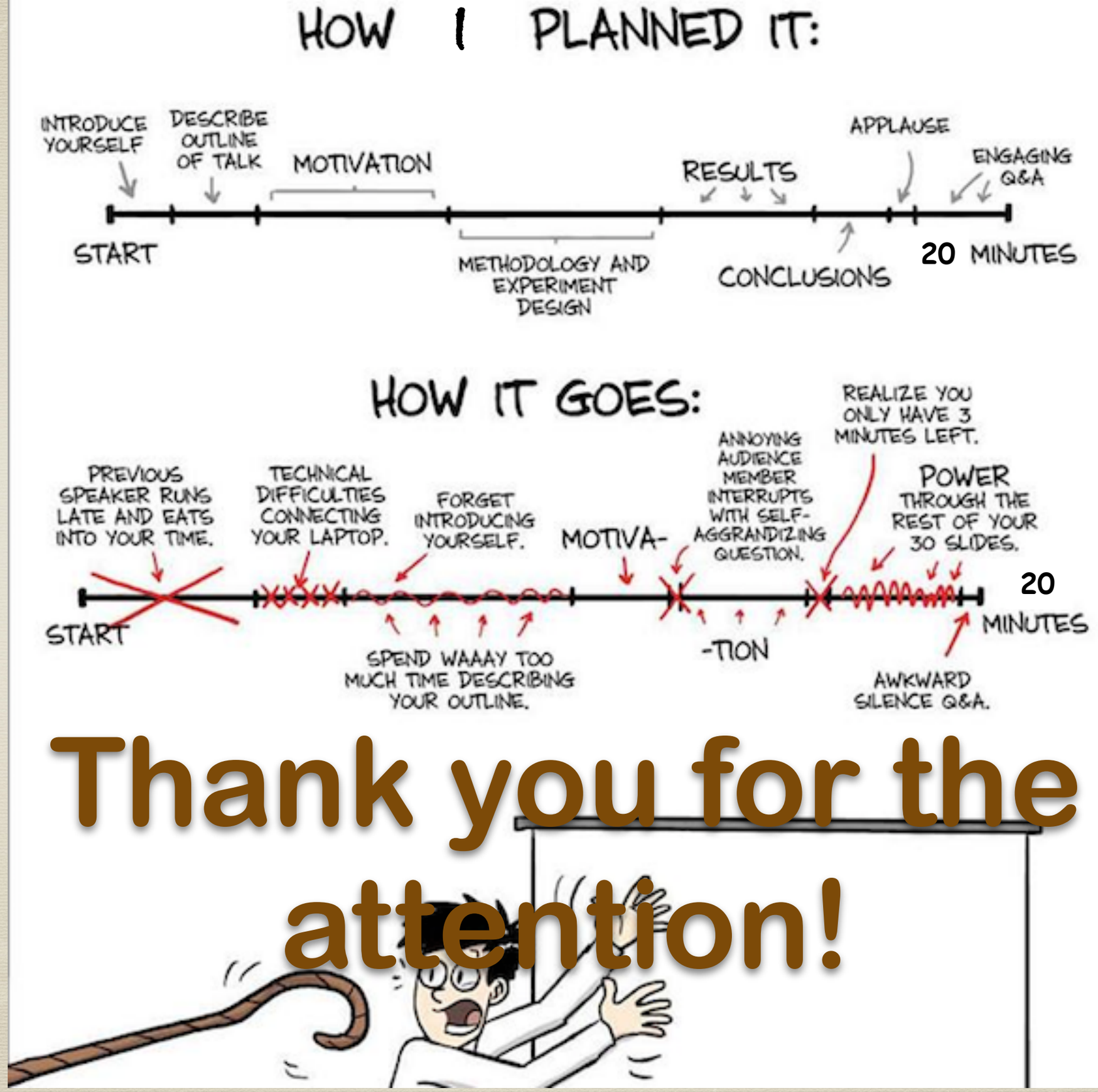
Summary results and works in progress

- **Parametrization of the equations of state (EOS) for Fe and SiO_2 up to pressures of 15 and 40 Mbar (abinit calculations);**

- **Extension of the EOS and the melting curve up to 1000 Mbar by both abinit and orbital free molecular dynamics (OFMD) calculations;**

- **Same for perovskite and post-perovskite ($MgSiO_3$)**

- **Use of results in hydrodynamic simulations and planetary modeling (sensivity?)**



Thank you for the attention!