Thermodynamical and transport properties of dense H-He mixtures

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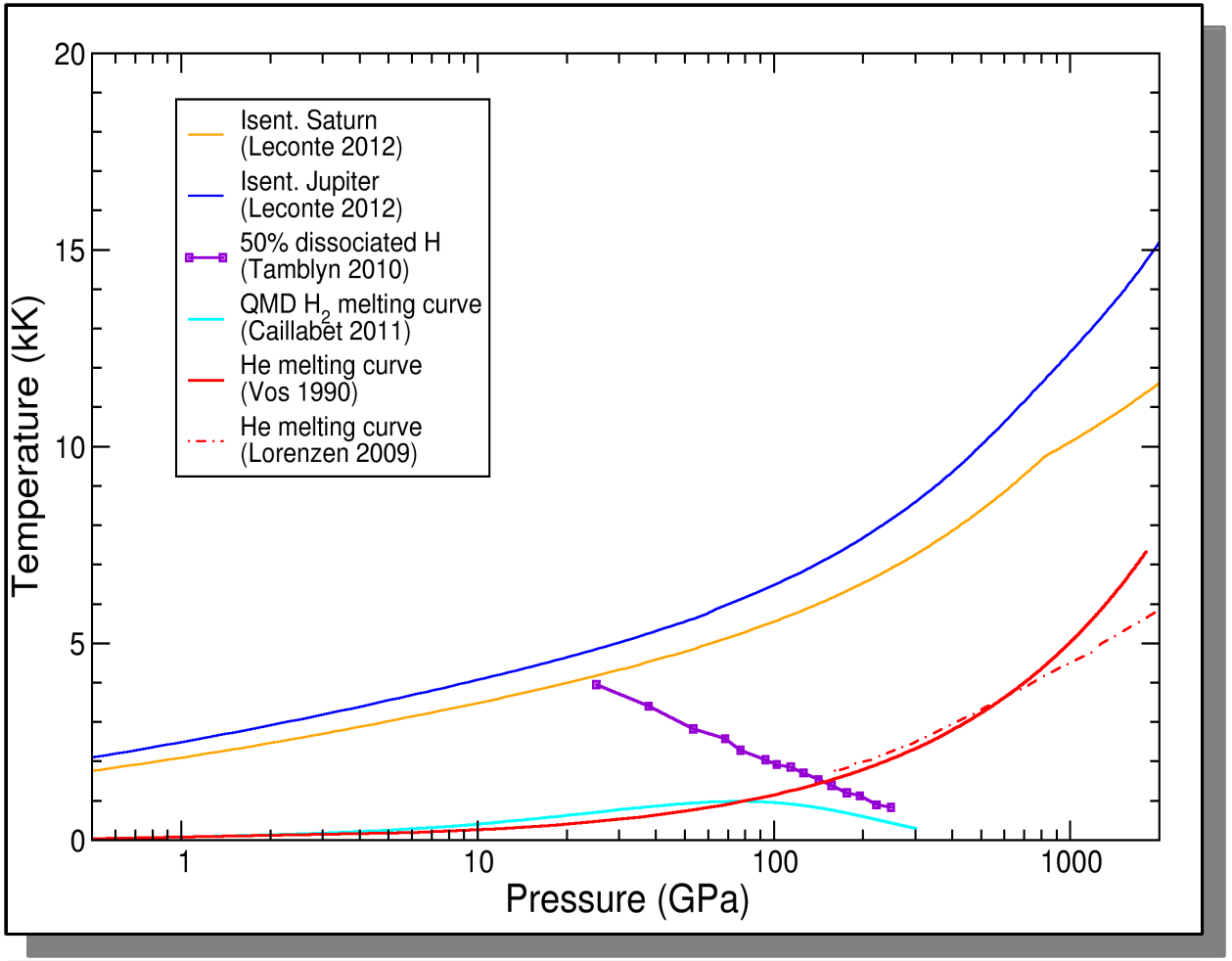
Introduction



Main phase transitions in pure H and He in the WDM regime overplotted on the P-T profiles for Jupiter and Saturn.

- Highly interesting for giant planets modeling.
- Phase transitions in pure systems (melting, dissociation, metalization).
- Influence in H/He mixtures?
- Phase separation in the mixture? Diagnostic?

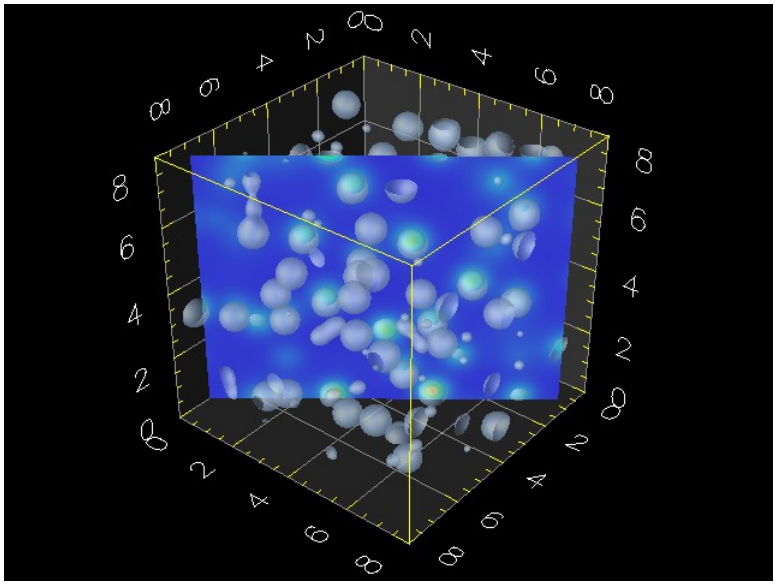
Numerical methods

- Quantum Molecular Dynamics (QMD) simulations with Abinit code.

- Equimolar H/He mixtures
  - ➔ To maximize the effects of the mixing

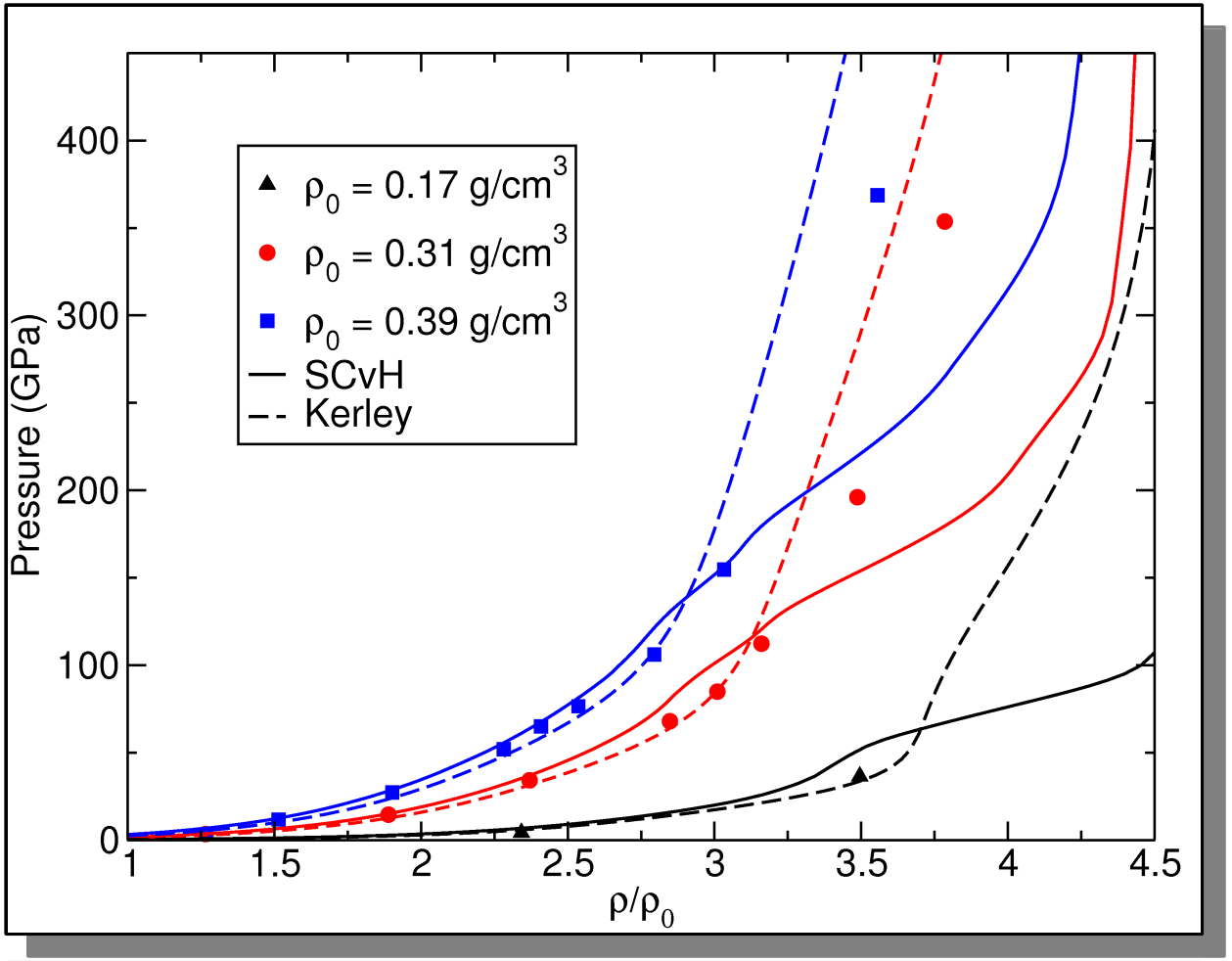
- 64 H – 64 He with periodic boundary conditions

- Time duration of about a few ps



Electronic isodensity surface: snapshot @ 1.19 g/cm^3 – 17405 K.

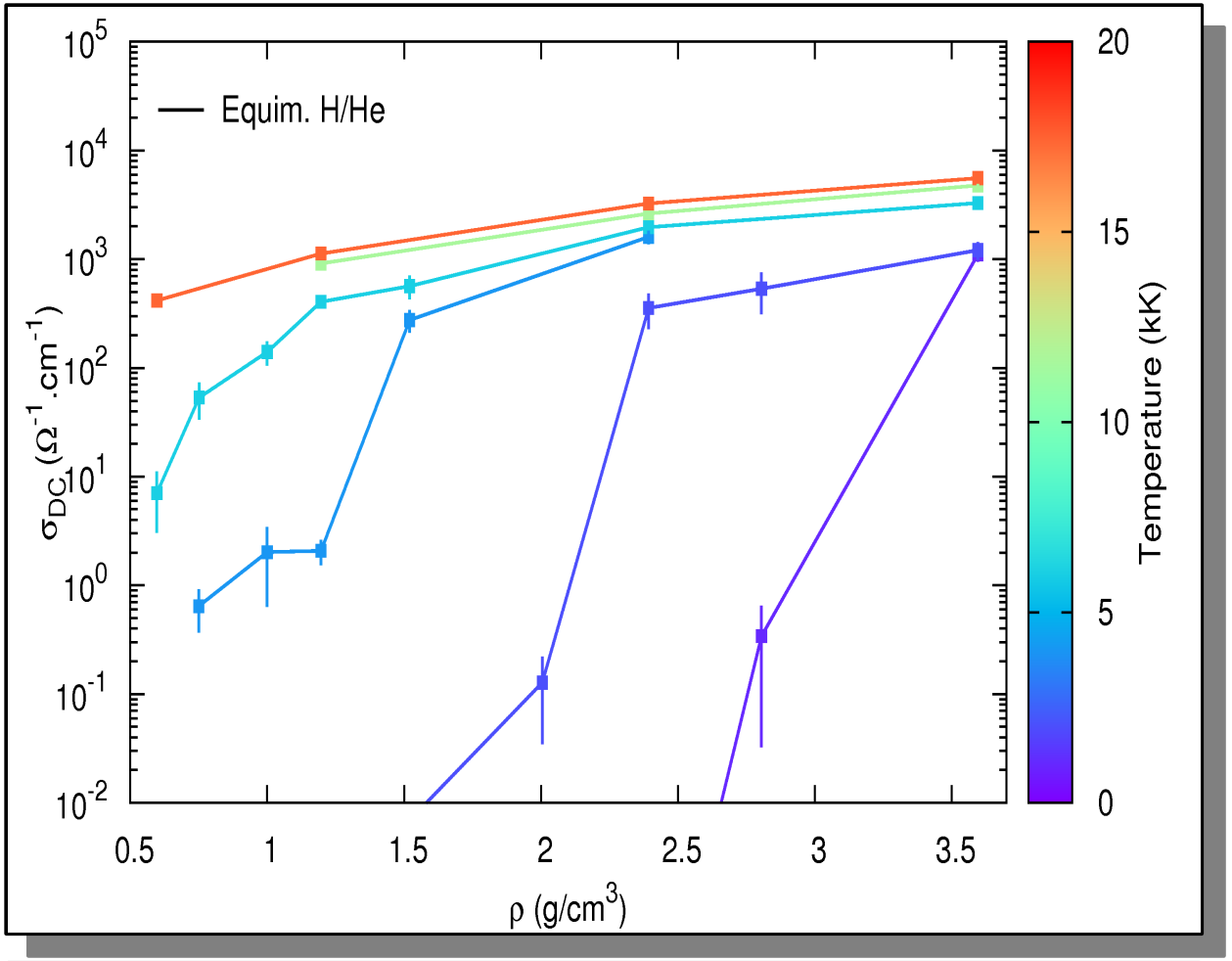
Thermodynamical properties



Hugoniot curves for equimolar H/He mixtures with different pre-compressed cells. Comparison with SCvH (1995) and Kerley (priv. com.) EOS predictions.

- QMD simulations provide the thermodynamics of the system (P, E at ρ, T).
- Predictions for Hugoniot curves.
- Close to Kerley prediction, SCvH more compressible.
- Should be compared to experimental results for validation.

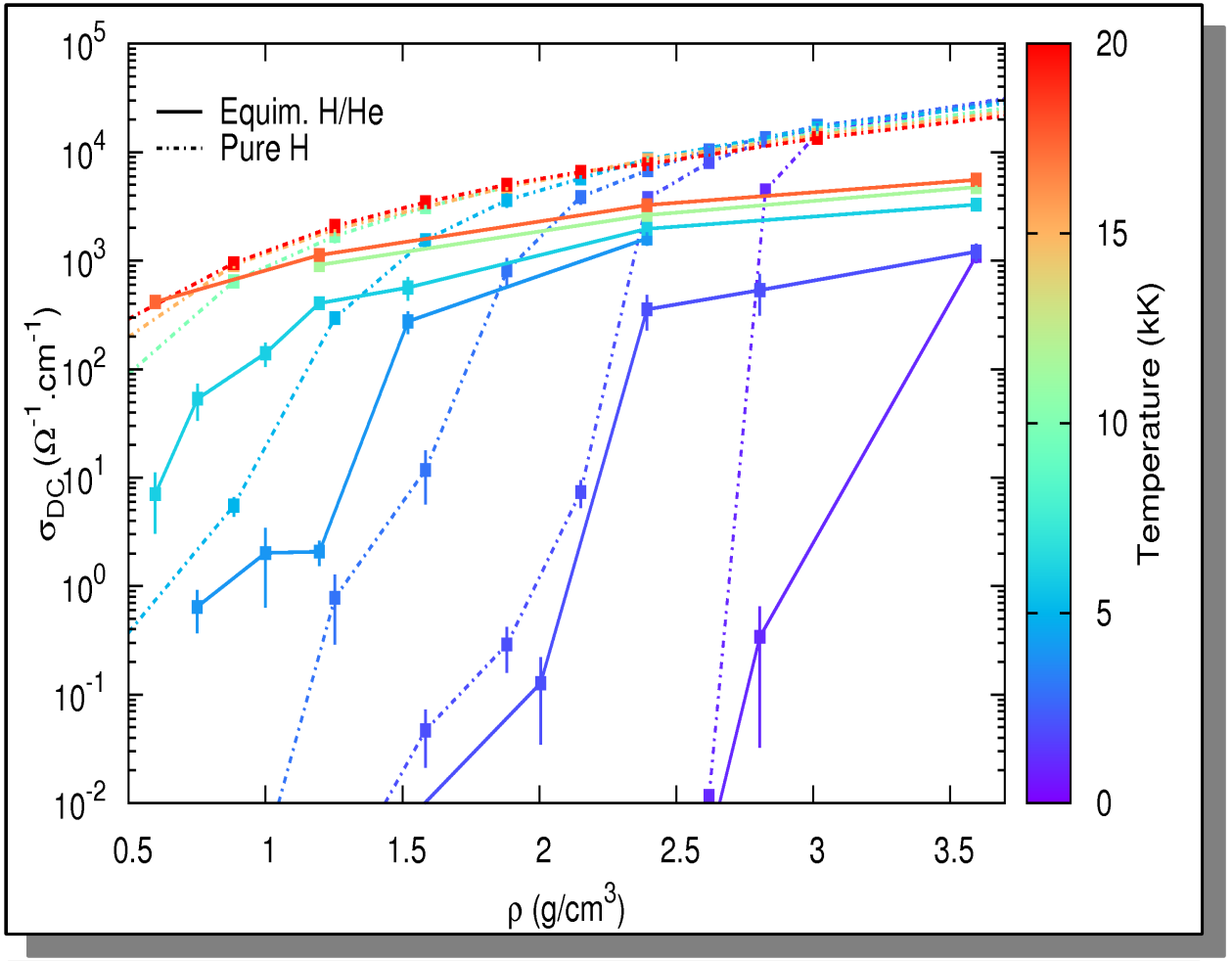
Transport properties



DC electrical conductivity isotherms of equimolar H/He (full line).

- Computation of the electrical conductivity in the mixture.
- Strong rise in conductivity at low temperature.

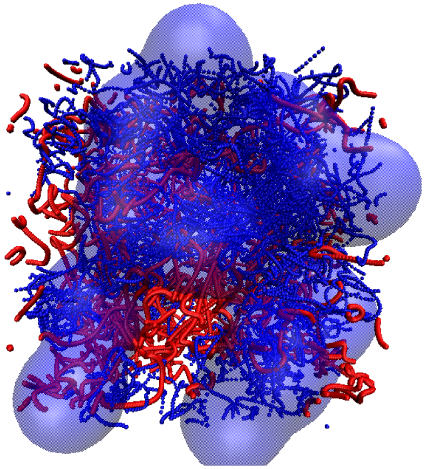
Transport properties



DC electrical conductivity isotherms of equimolar H/He (full line) and of pure H (dashed-dotted line) computed by Holst *et al* (2011) but plotted as a function of an effective density in a fictitious H/He equimolar mixture with an He steric volume of (0.9 Å)^3.

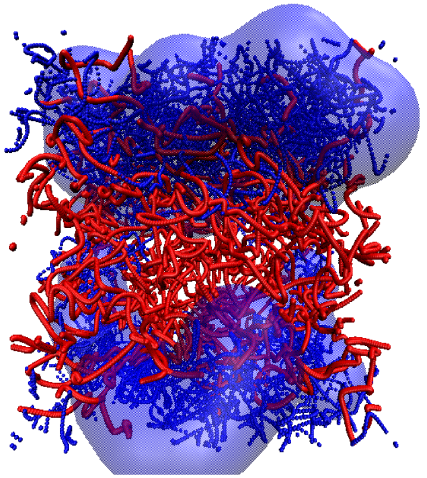
- Computation of the electrical conductivity in the mixture.
- Strong rise in conductivity at low temperature.
- Fully compatible with pure H results assuming a steric effect of He with a volume of (0.9 Å)^3.
- Lower plateau at high density than in pure H systems.

Phase separation: observation



Homogeneous **state.**

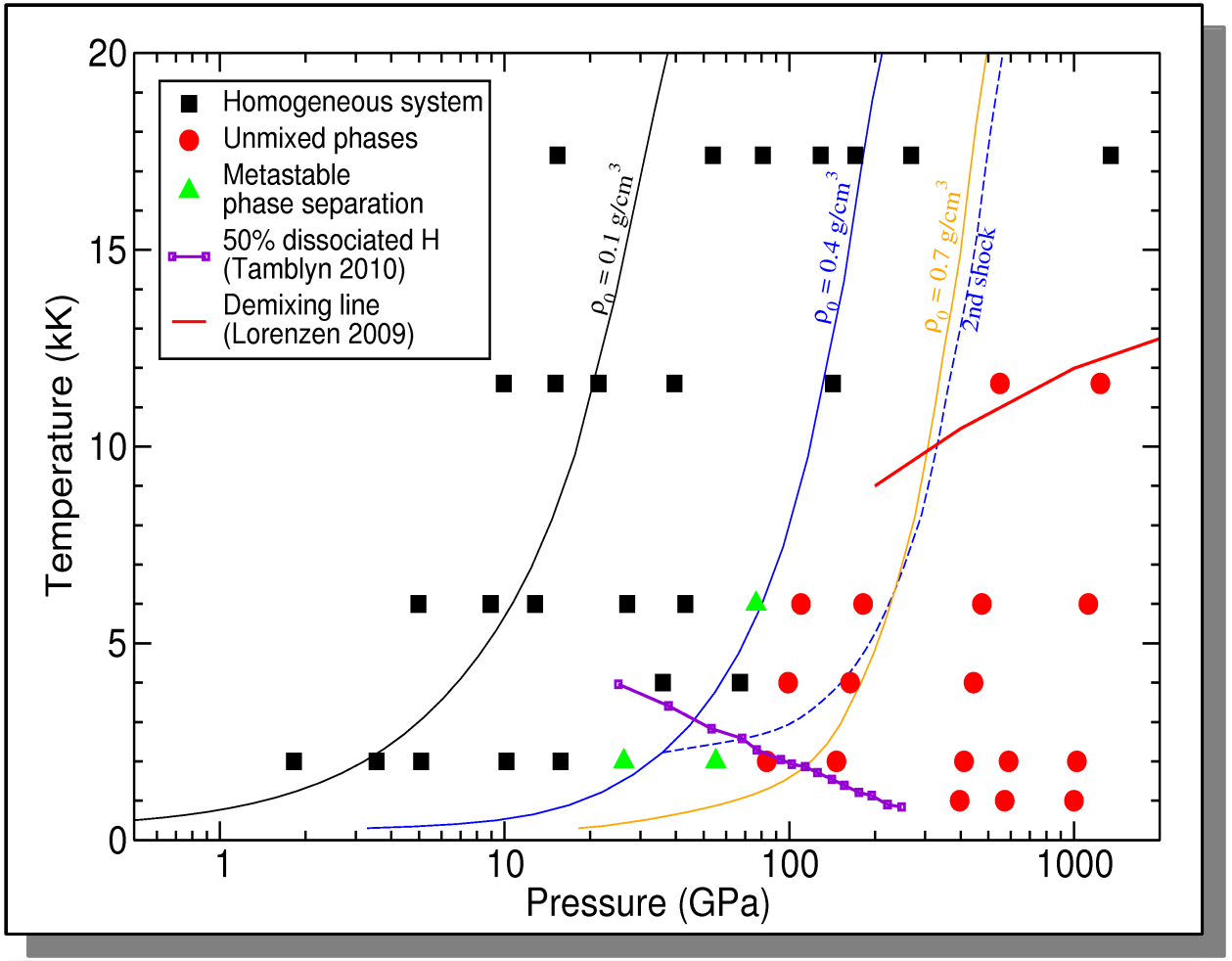
Isodensity surfaces snap-shot for H in transparent blue. Trajectory of H (resp. He) nuclei in blue (resp. red) over 400 time steps of the MD.
Equimolar H/He mixtures @ 1.5 g/cm^3 – 4000 K.



Inhomogeneous **state.**

- Observation of the trajectory of the nuclei in the simulation box.
- Transition from a whole space occupation state to a partial occupation state
  - ➔ Phase separation
- "Natural" transition quite independent of the initial conditions
- Observed in 512 particles simulation
  - ➔ Limited finite size effects

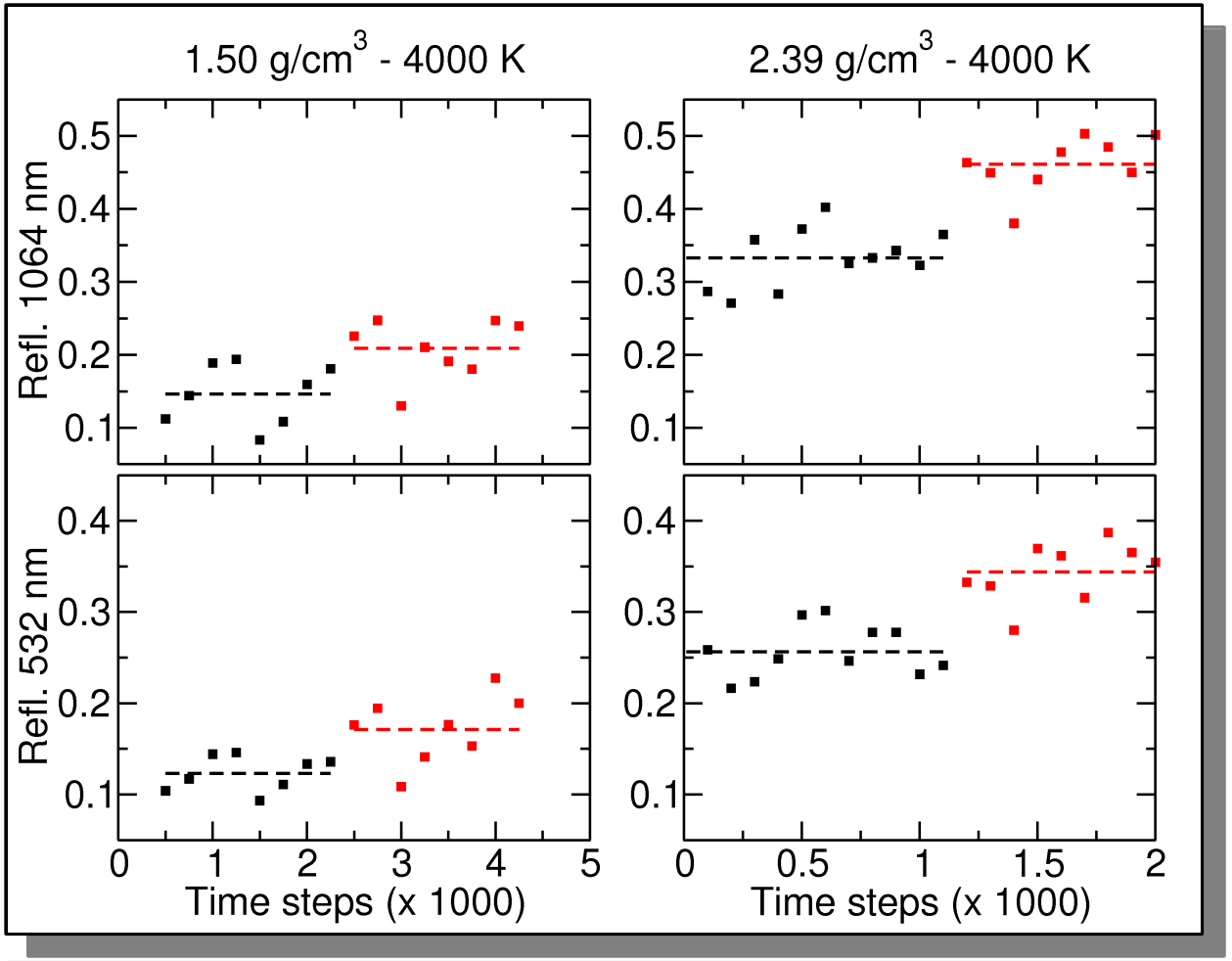
Phase separation: diagram and accessibility



Estimated phase diagram for an equimolar H/He mixture. Tamblyn's dissociation line in pure H (violet) and Lorenzen's demixing line computation (red) are plotted. The other full lines are hugoniot curves prediction (with SCvH 1995) with different initial precompression. The blue dotted line represents a second shock curve initiated from the 0,4gcc hugoniot at 30 GPa.

- Estimated phase diagram.
- Compatible with Lorenzen et al predictions.
- Need high precompression to be reached in laser-driven experiment or second shock technique.
- Diagnostic?

Phase separation: reflectivity diagnostic



Time evolution of the reflectivity at 532 and 1064 nm in two MD simulations presenting a transition to demixion. In black the system is homogeneous, in red it is separated.

- Computation of the reflectivity during the simulation.
- Significant rise in reflectivity.
- Synchronized with the observed phase separation.
- We should be able to make the difference in laser-driven experiments → diagnostic.

Conclusion

- QMD simulations of equimolar H/He mixtures in the WDM regime.

- Extraction of some thermodynamical properties but limited access to the entropy.

- Computation of the electrical conductivity: steric role played by He on the metalization/dissociation of H.

- Observation of a phase separation during the simulation.

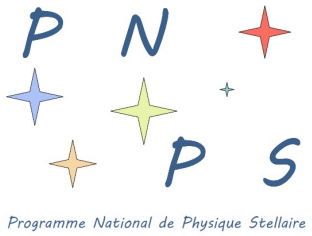
- Possible diagnostic of the phase separation in laser-driven experiments
  - ➔ Reflectivity of the mixture

- Waiting for experimental results...

- May have a strong impact on the giant planets modeling.

Acknowledgments

- ***Fundings:***



- ***Computation facilities:***

THANK YOU!