AB INITIO PERSPECTIVE ON

GIANT IMPACTS AND PROTOLUNAR DISKS

RAZVAN CARACAS

CNRS, ENS LYON

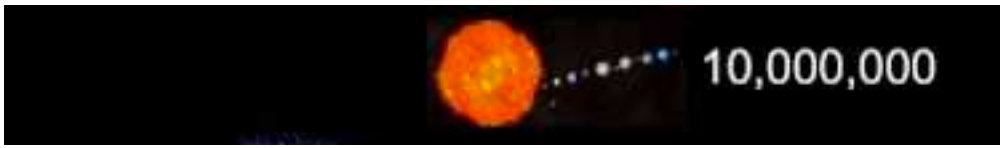
Laboratory Of Geology Of Lyon & Centre Blaise Pascal

In collaboration with Sarah T. Stewart (UC Davis),
and the IMPACT team: Ema Bobocioiu, Anais Kobsch, Zhi Li, Natalia Solomatova

https://moonimpact.eu/

10^{21}

10^{15}



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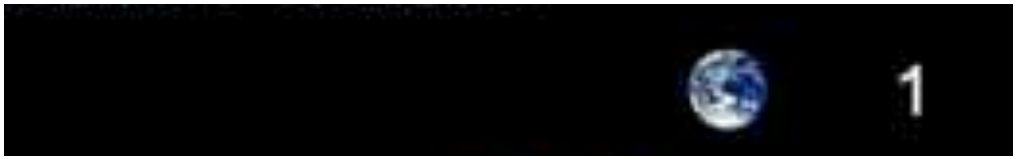

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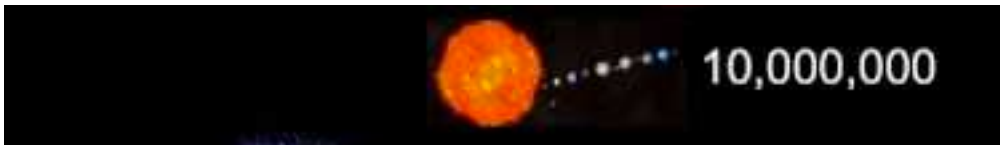

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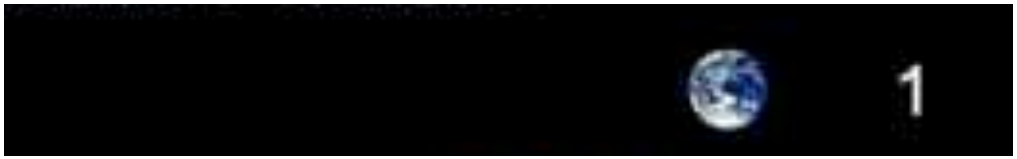

10^{0}

I am in the basement at $10^{-15 .. -21}$

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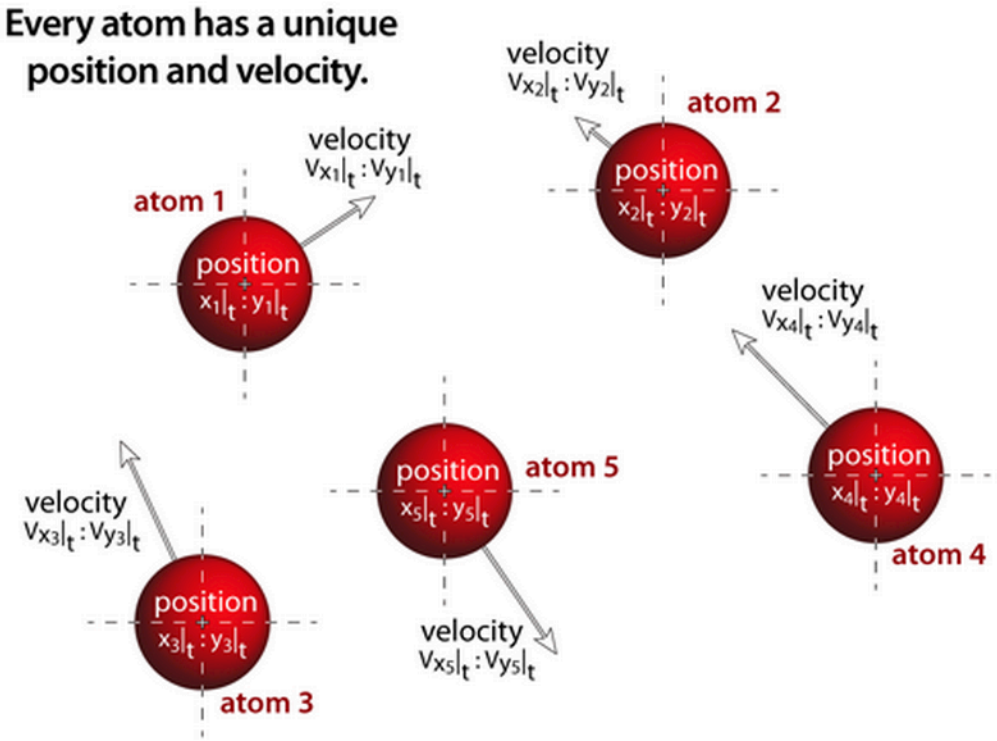
TOOLS:

- first-principles molecular dynamics (AIMD, NVT, DFT, PAW, GGA, etc.)
  to study liquids, gases, supercritical fluids
- maximum of liquid-gas separation defines the super-critical point
- pure terms, complex phases, presence of volatiles

PROPERTIES:

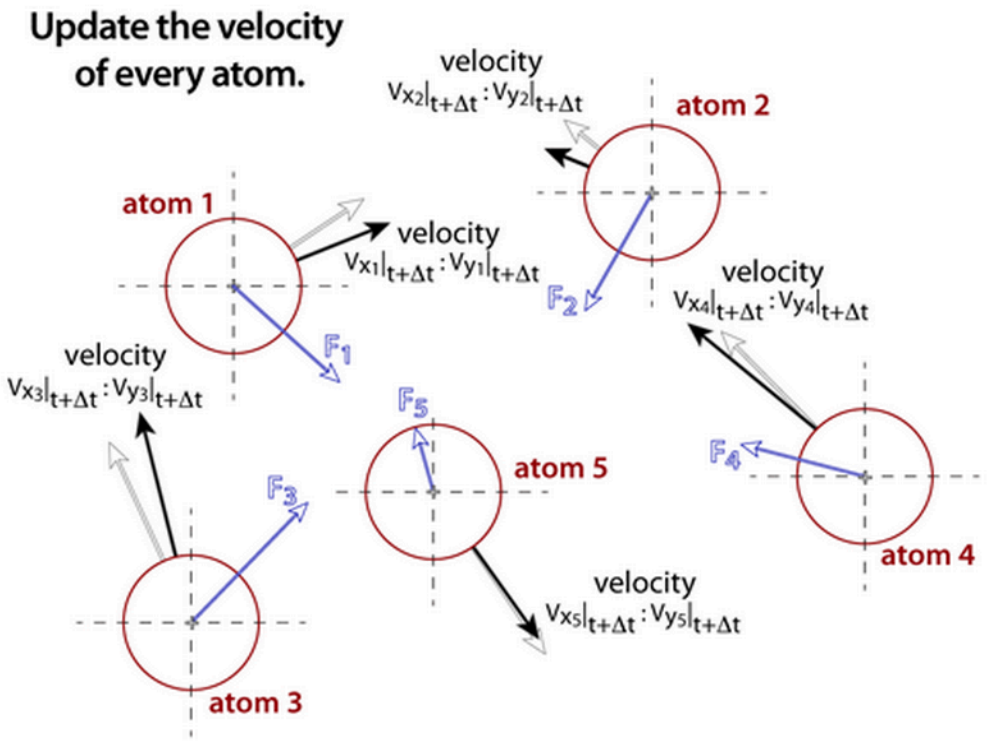
- SUPERCRITICAL POINT & DOME
- liquid/gas equilibrium
- equation of states, speciation, element and isotope partitioning
- electronic (i.e. optical) properties, disk opacities, vibrational spectroscopy



step 1

Every atom has a unique position and velocity within the simulation, and all of the atomistic properties associated with that specific atom: atomic name, atomic mass, atomic radius, and the interatomic potential functions. All of the atoms are treated as if they are classical particles that move according to Newton's laws of motion (*i.e.* F=ma; thus, the acceleration (a) acting on any atom is determined by the net interatomic force (F) acting on the the atom divided by the atom's mass (m)).

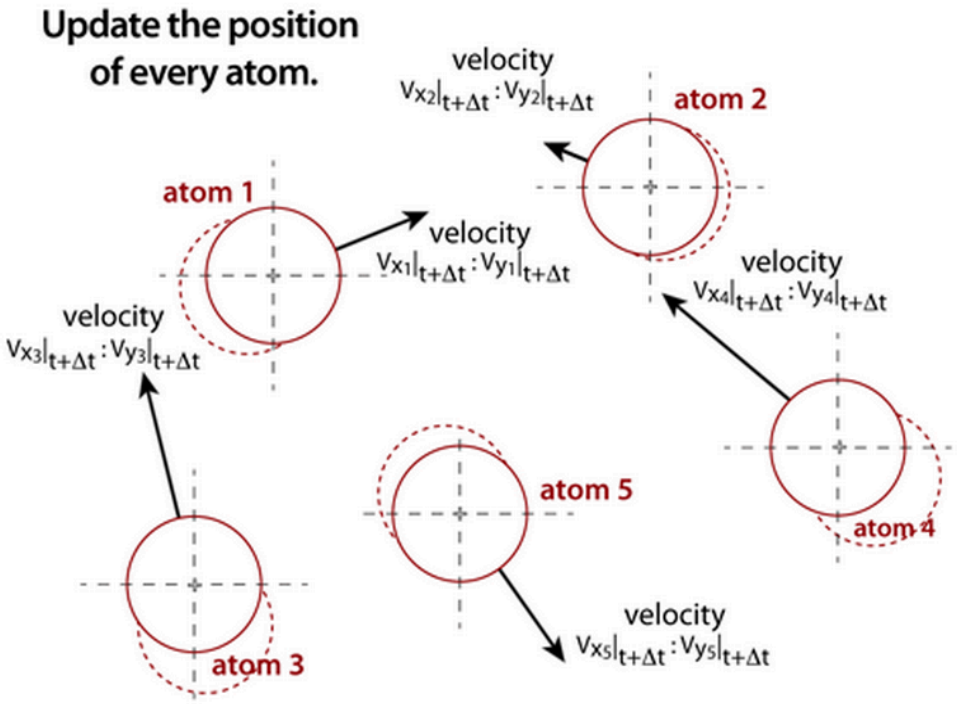
http://atomsinmotion.com/book/chapter5/md



step 5

Once the net force on each of the atoms is known, the velocities can be estimated from Newton's law assuming that the forces are constant over a small enough increment in time. The time steps in molecular dynamics simulations are very small, typically between femtoseconds ($1fs = 1x10^{-15}$ s) and picoseconds ($1ps = 1x10^{-12}$ s). Essentially, the acceleration on the atom is multiplied by the time step to determine the change in velocity. After all of the velocities are determined, a thermostat is used to scale the velocities in such a way that the appropriate energy of the system is maintained.

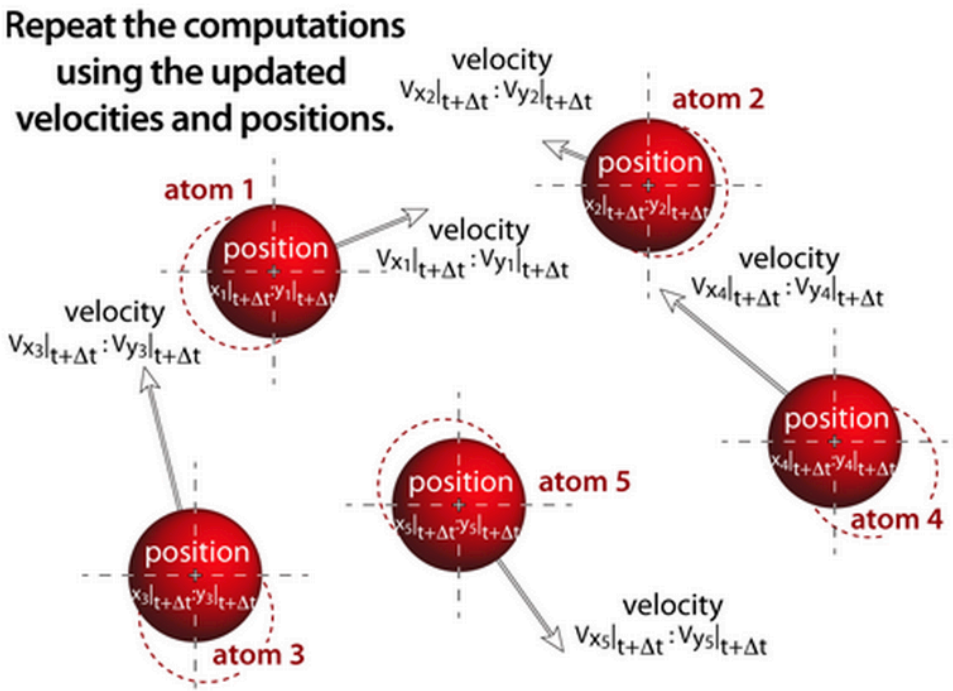
http://atomsinmotion.com/book/chapter5/md



step 6

The positions of each atom must also be updated. Once the net forces that are acting on the atoms are known, then the positions of each atom can be updated through very accurate integration algoritms. These integrators, such as the Verlet or Leap-Frog algorithms, will increment the position of an atom from its current position based on the net force, velocity, and time step. The integration methods, thermostats, and time steps must be selected based on compromises between accuracy, stability, and speed.

http://atomsinmotion.com/book/chapter5/md

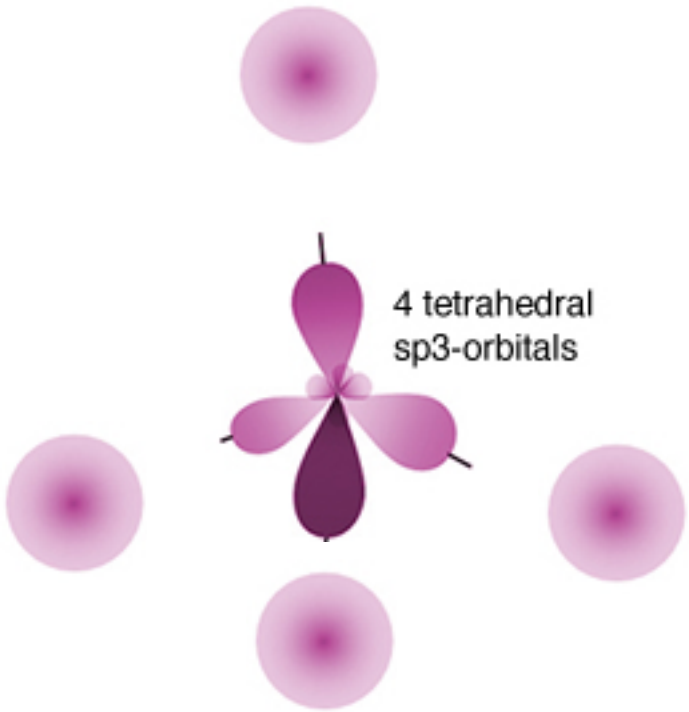


step 7

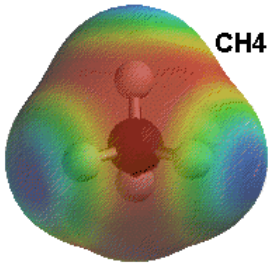
Molecular dynamics experiments proceed iteratively, where the output from one iteration becomes the input to the next (*i.e.* this step now becomes step 1 and the process repeats!). The above sequence of steps represents the computational process that occurs numerous times before the atoms are rendered to the screen. In these simulations, this computational loop will actually be repeated 5-20 times (depending on the number of atoms within the simulation) before the atoms are drawn to the screen. As the number of atoms in the simulation increases the time it takes to compute the new positions and velocities also increases. And in an effort to keep the simulation interactive, the atoms are drawn more frequently as the simulation size increases; this results in the atoms appearing to move more slowly as the number of atoms increases — *an unavoidable consequence of complex "real-time" computational simulations*.

Timesteps ~ 1 femtosecond

Statistics after ~ ten(s) of picoseconds

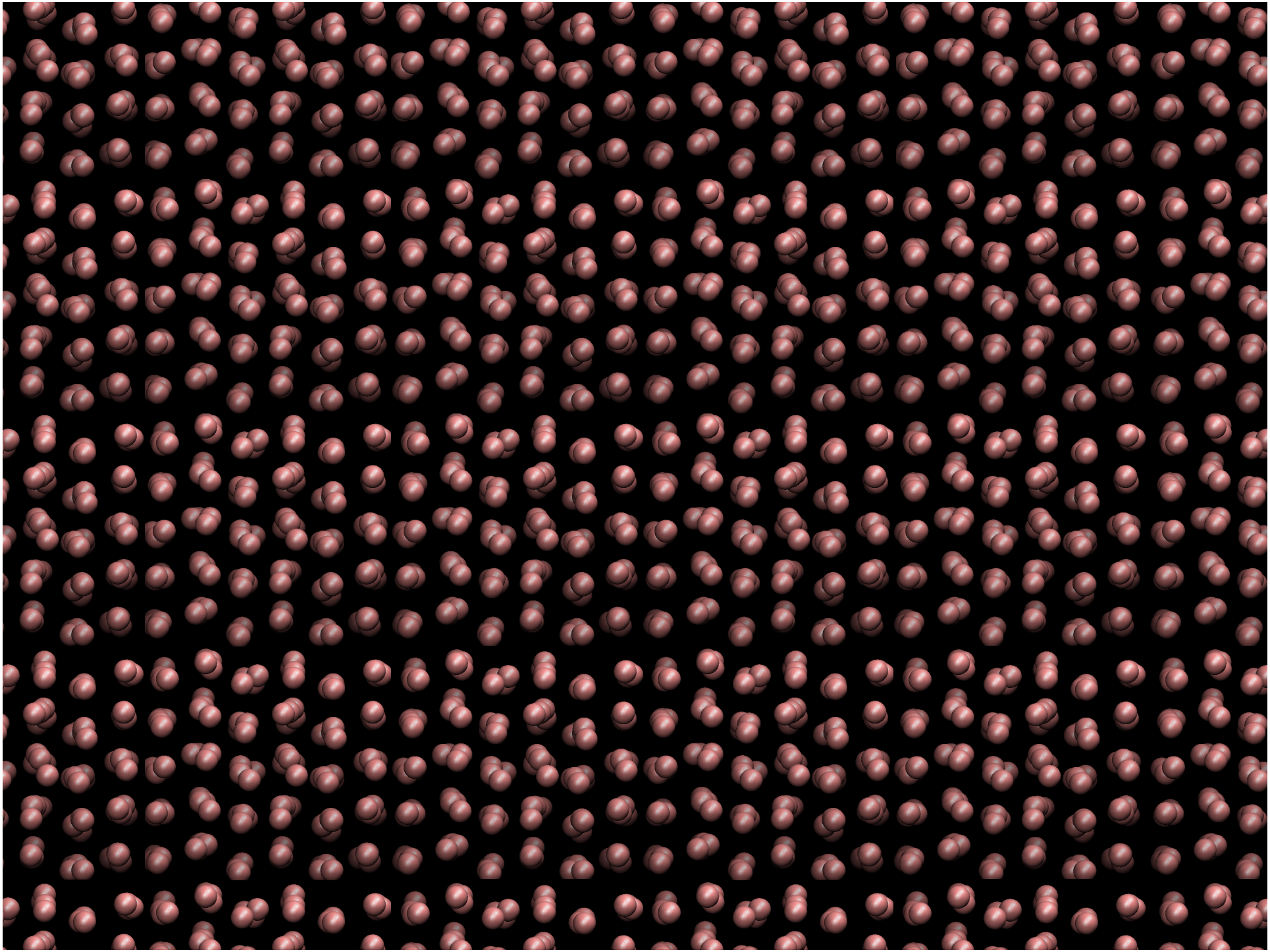


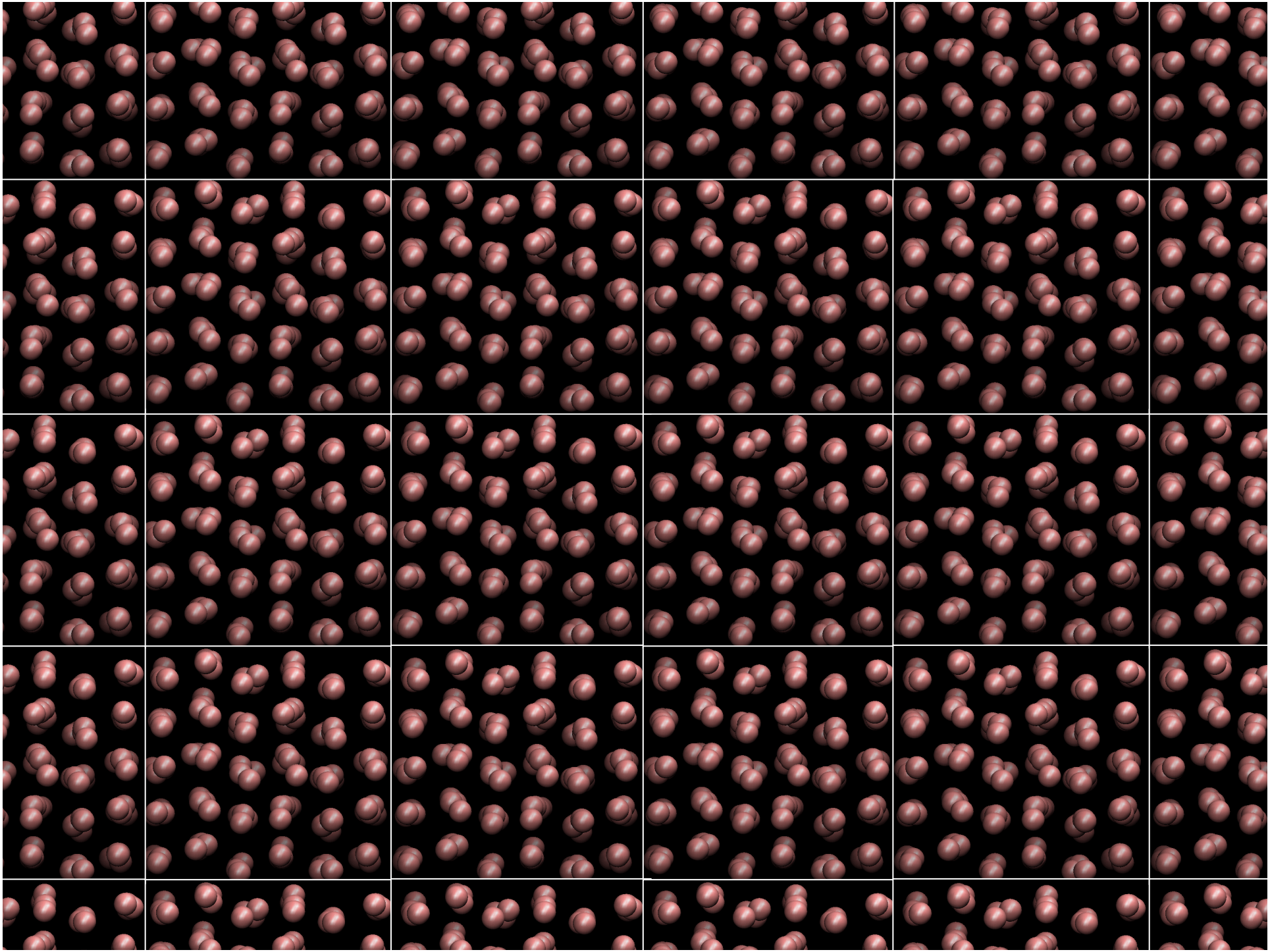
Density
Functional
Theory



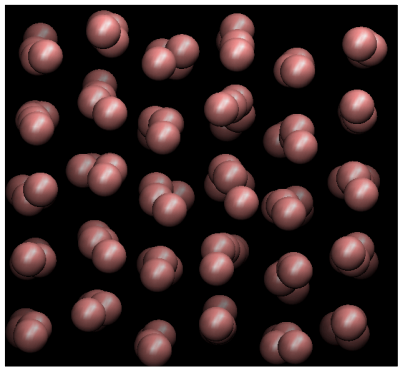
ENERGY + CHARGE

ALL PHYSICAL PROPERTIES





PROCEDURE



We calculate the

forces acting on the atoms

=>

From there we obtain velocities

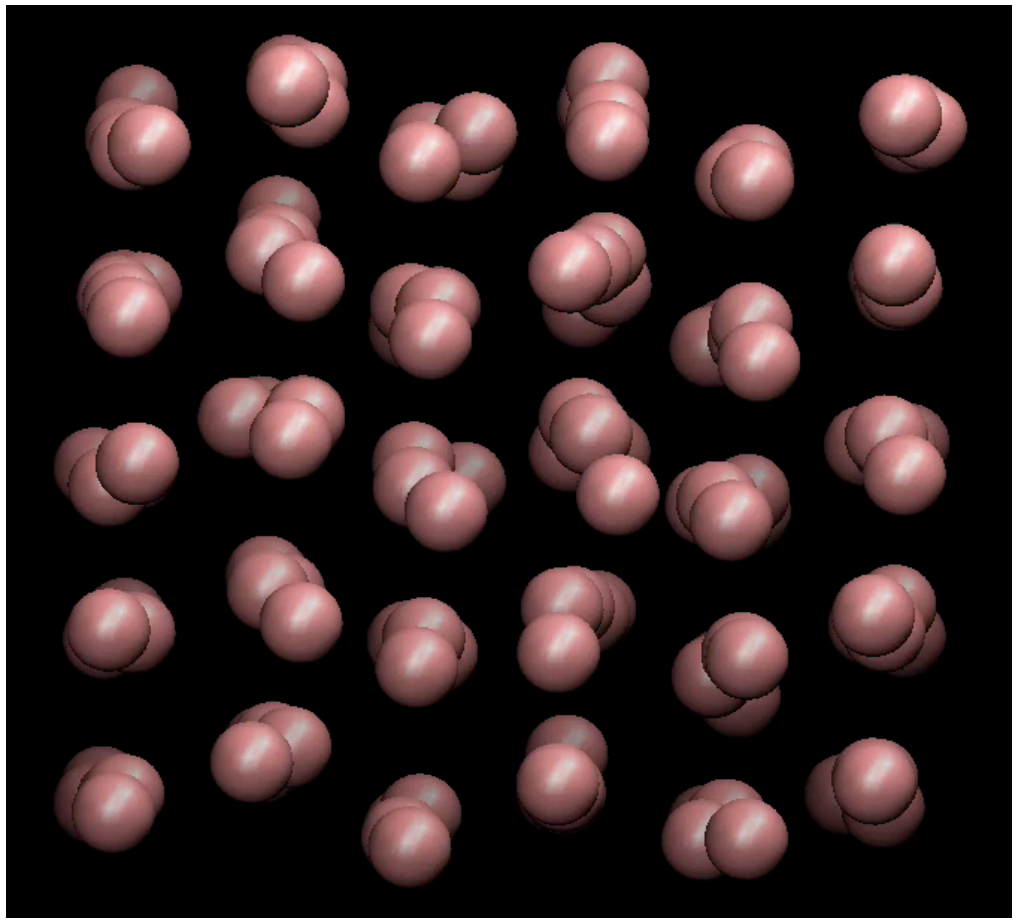
=> thanks to Newton,

We calculate the new positions

Time step on the order of 1 fs (1 femtosecond = 10^{-15} seconds !!!!)

PROCEDURE

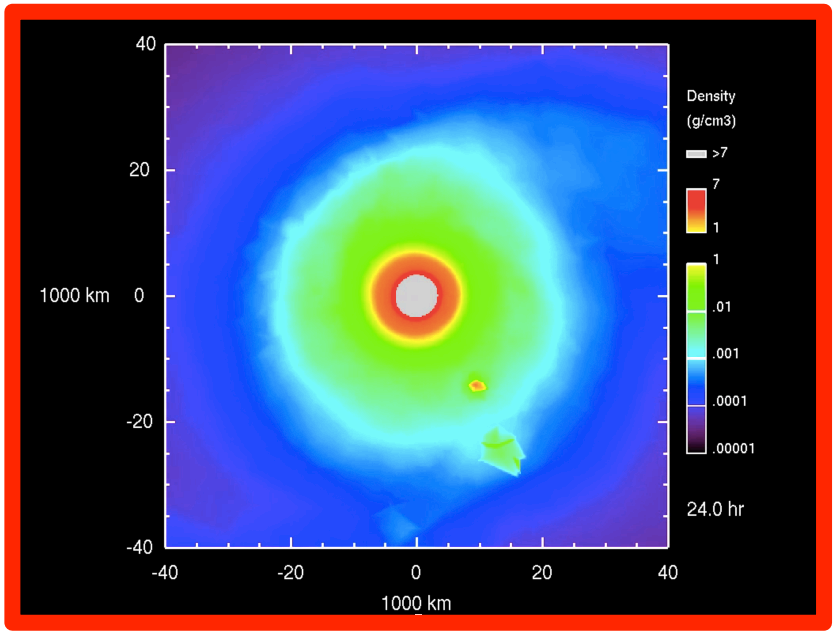
We start with a snapshot of a vibrating solid and heat it up until it melts.
Overheating!
Velocity of moving atoms scales with temperature.



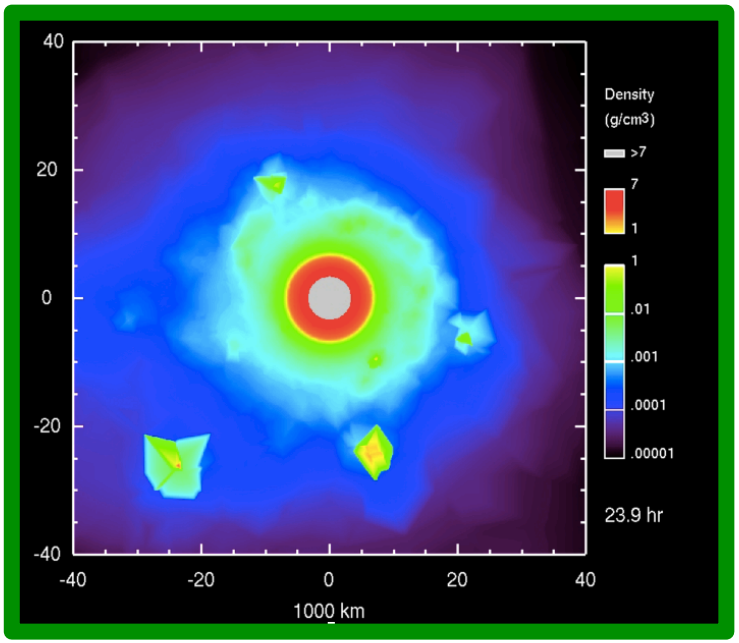
Simulation time on the order of a few ps

(1 picosecond = 10^3 femtoseconds)

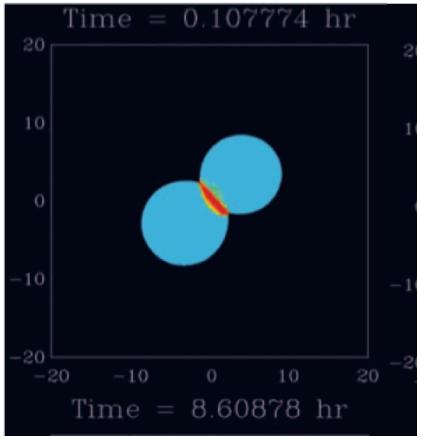
THE GIANT IMPACT



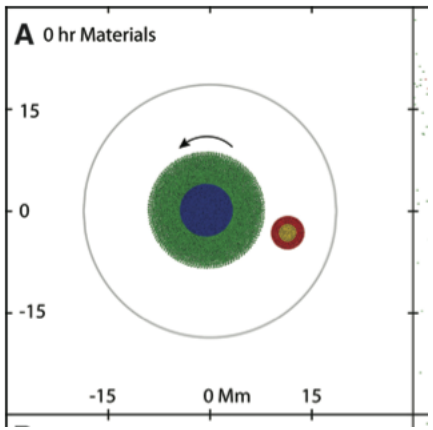
similar sized impactor and proto-Earth



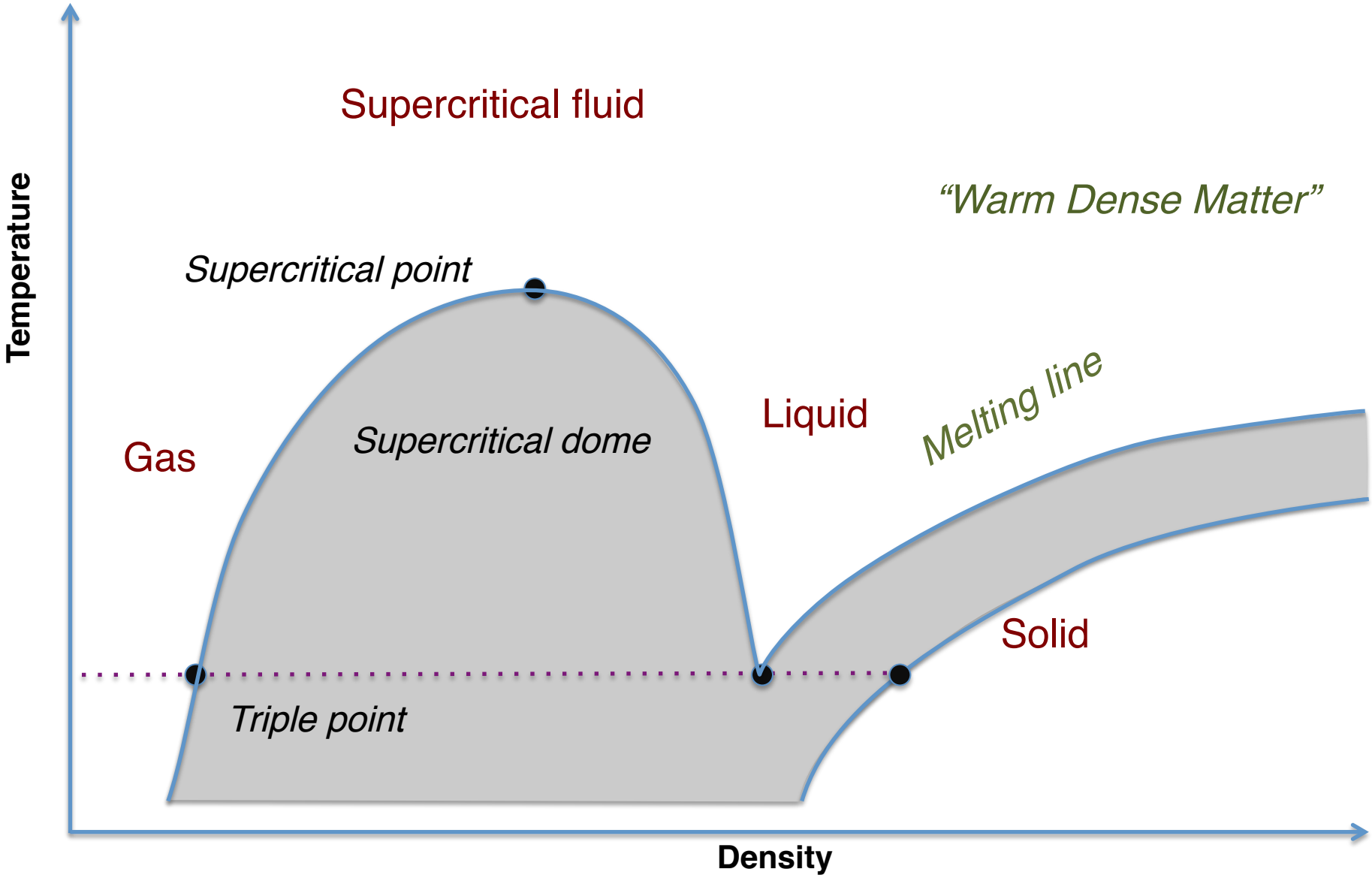
fast-spinning large proto-Earth + small impactor

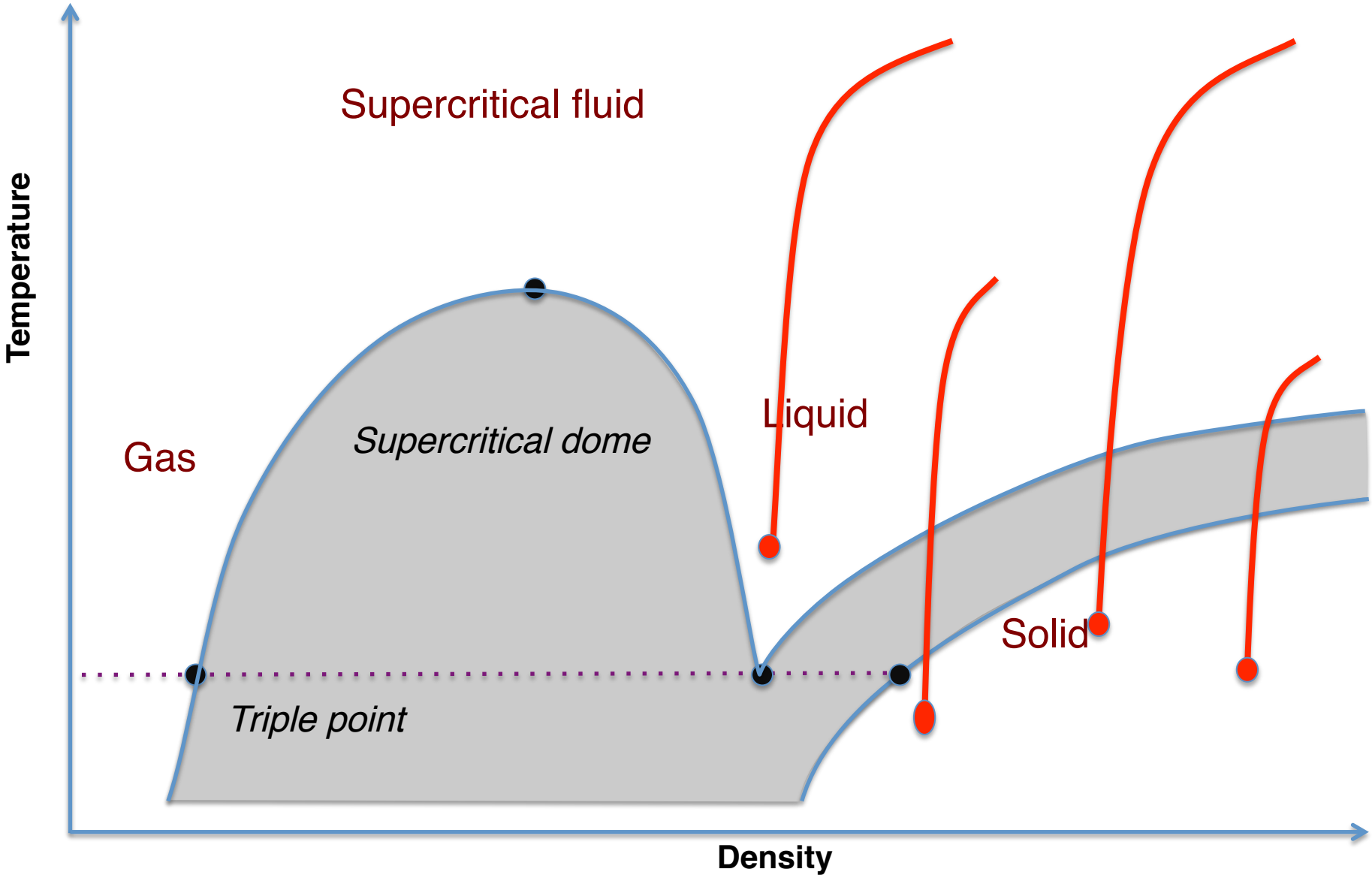


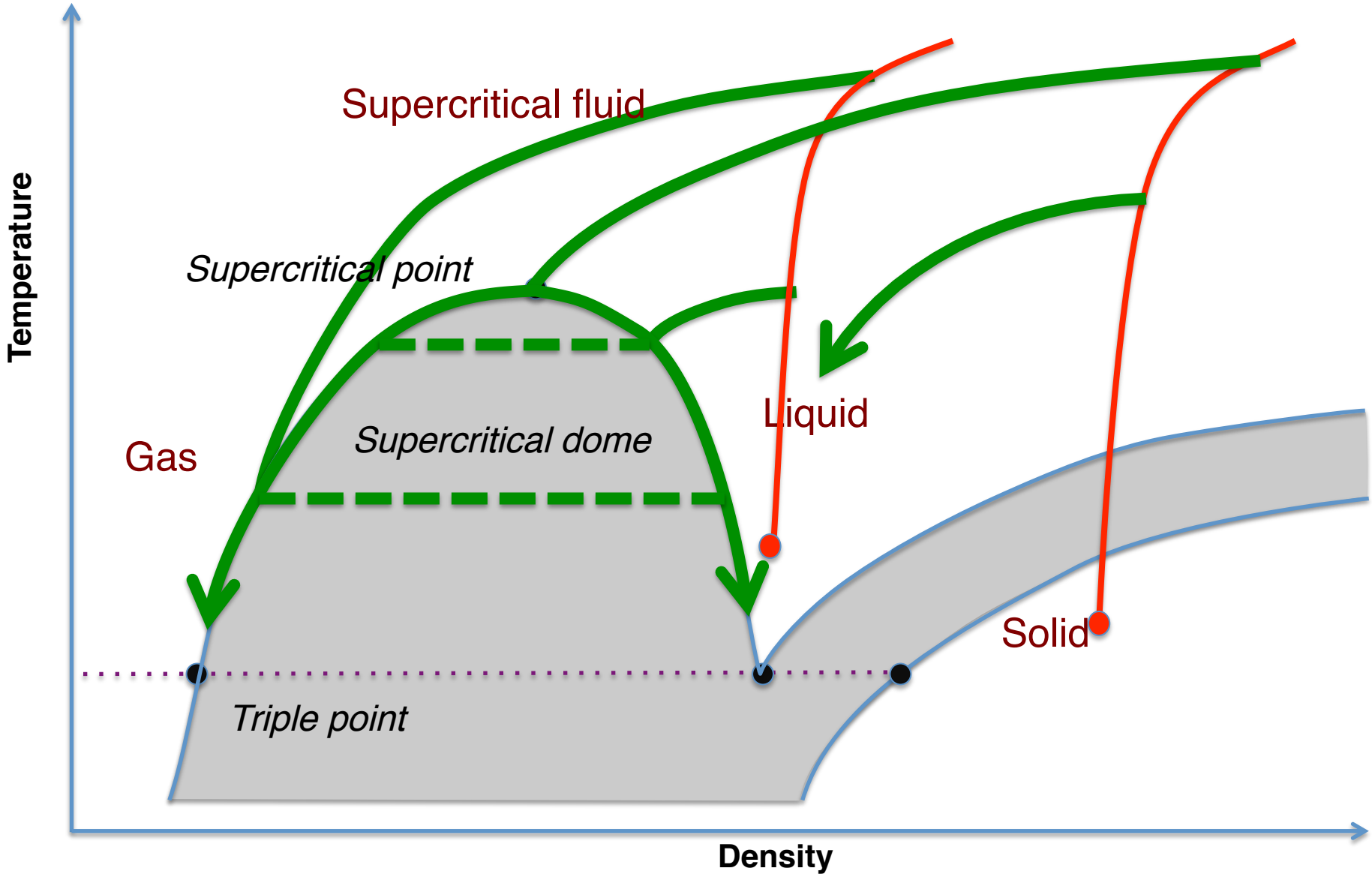
Canup et al., Science 2012

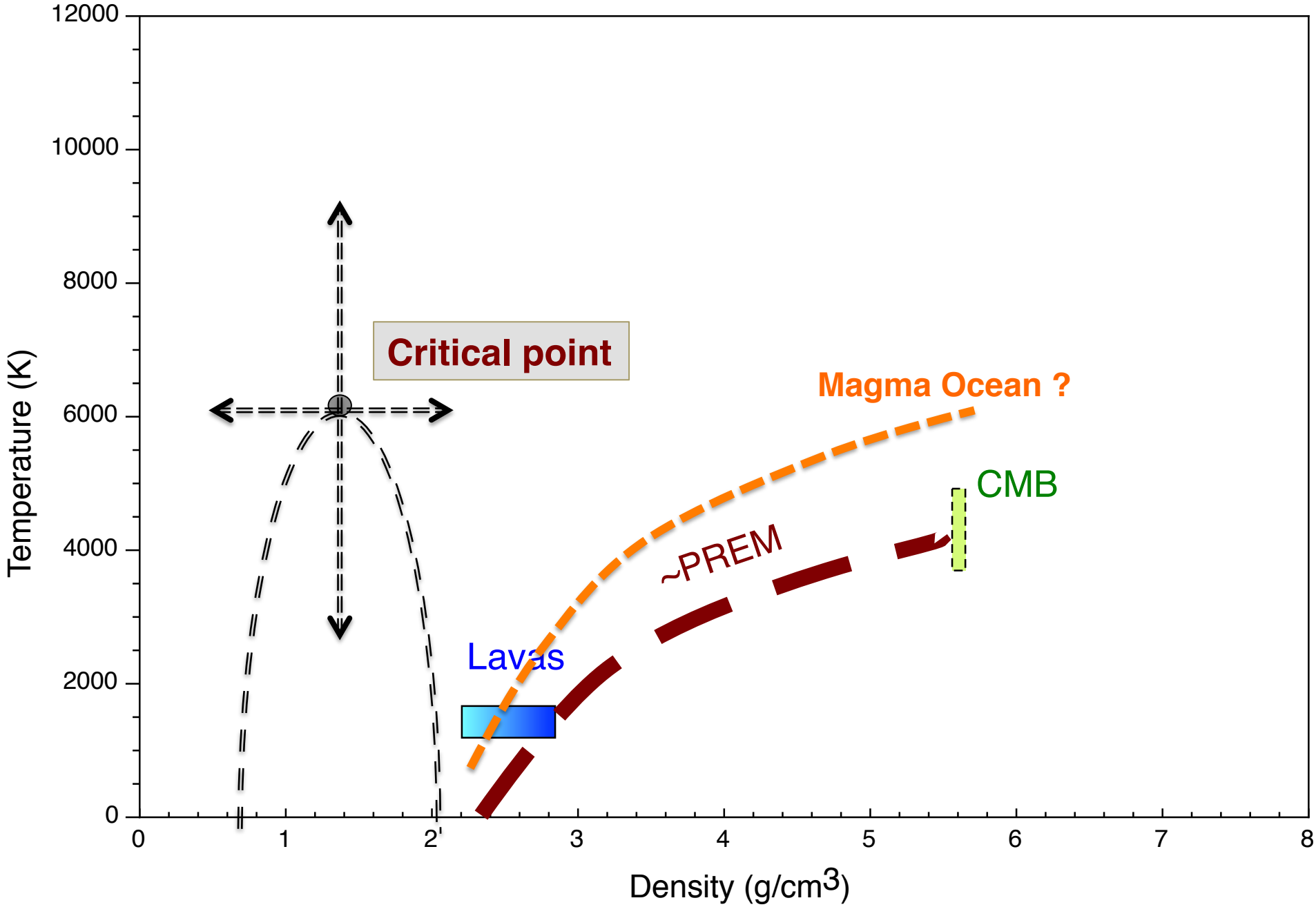


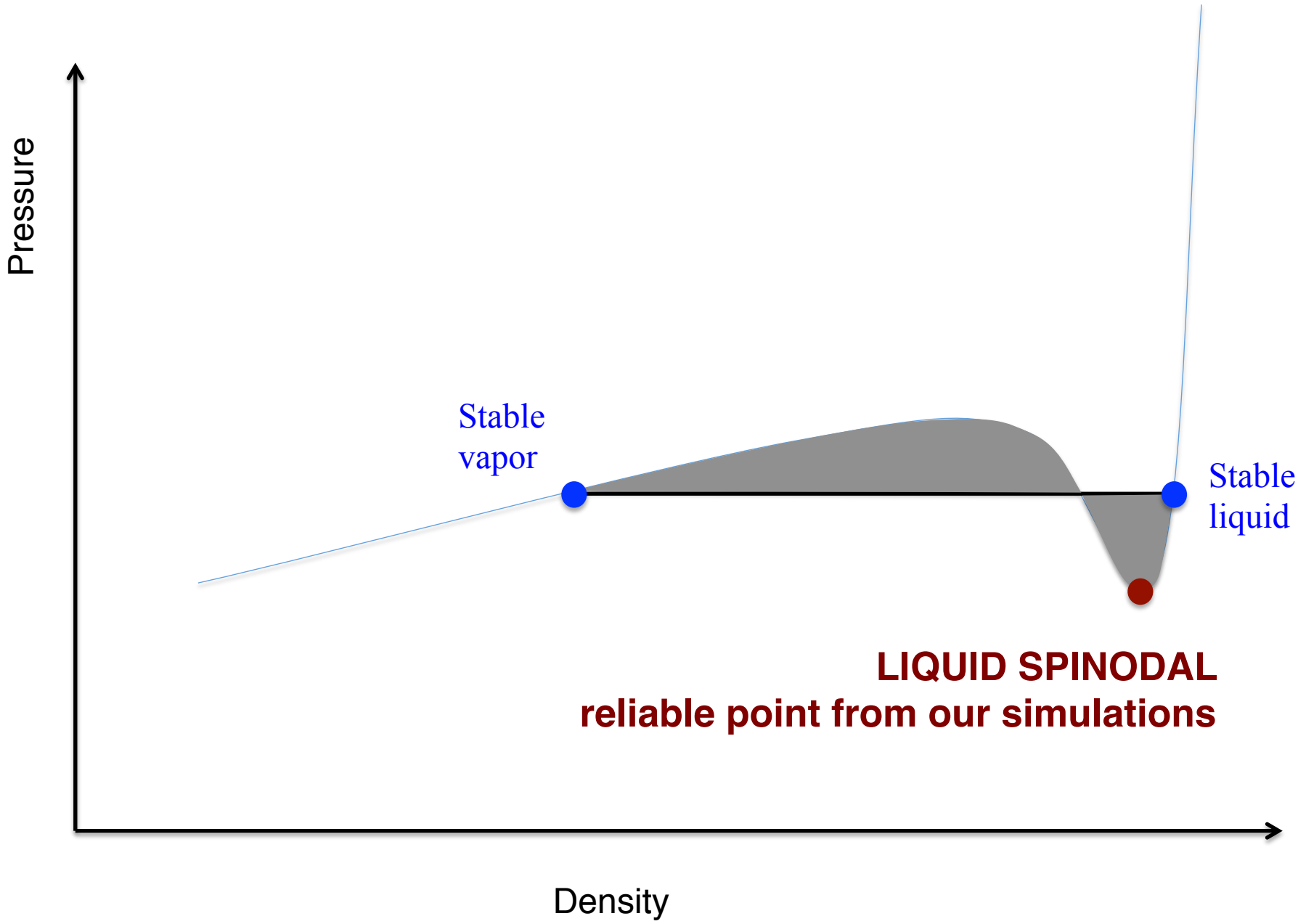
Ćuk and Stewart, Science 2012

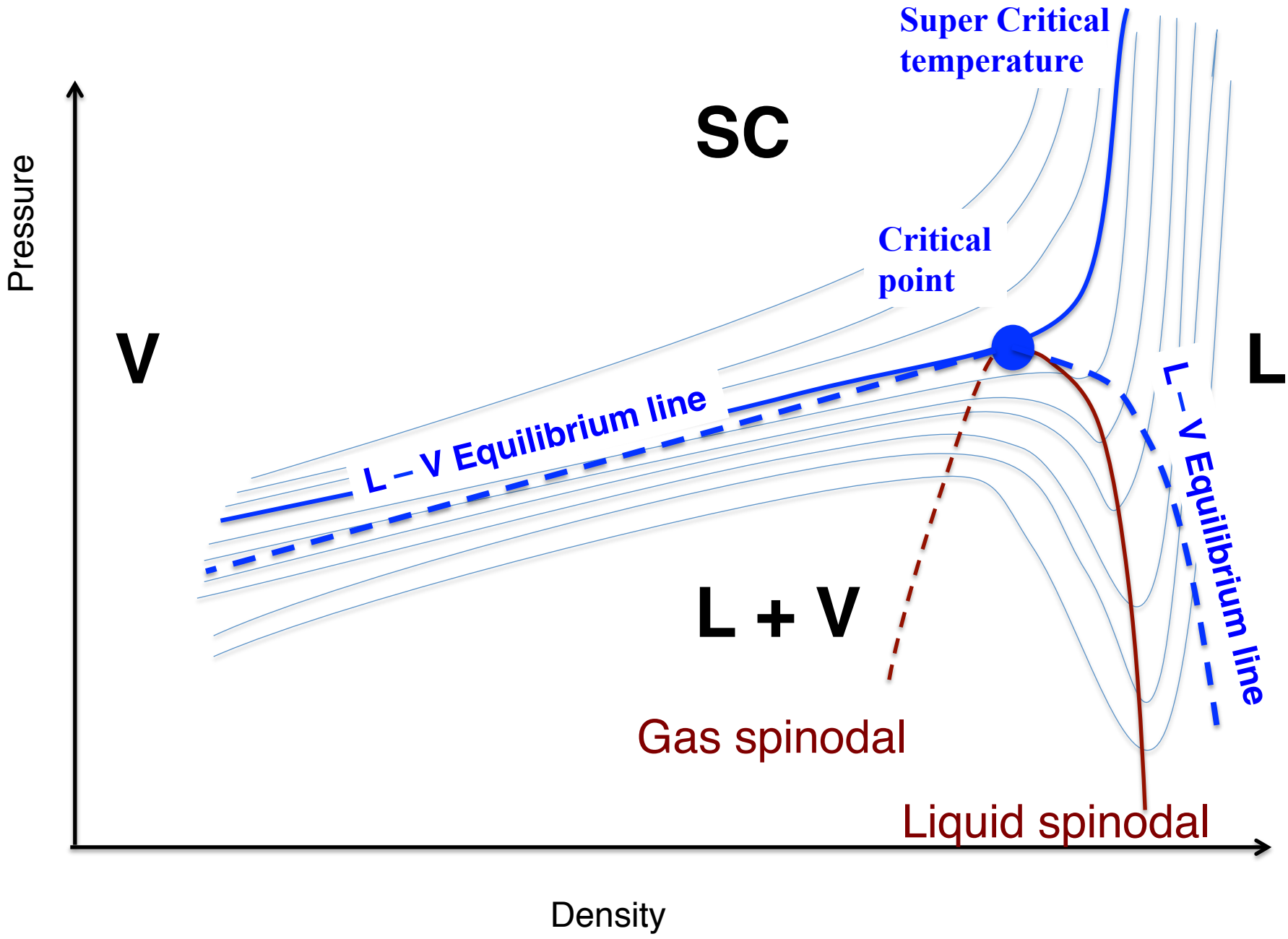

Supercritical fluid
"Warm Dense Matter"
Supercritical point
Temperature
Gas
Supercritical dome
Liquid
Melting line
Solid
Triple point
Density

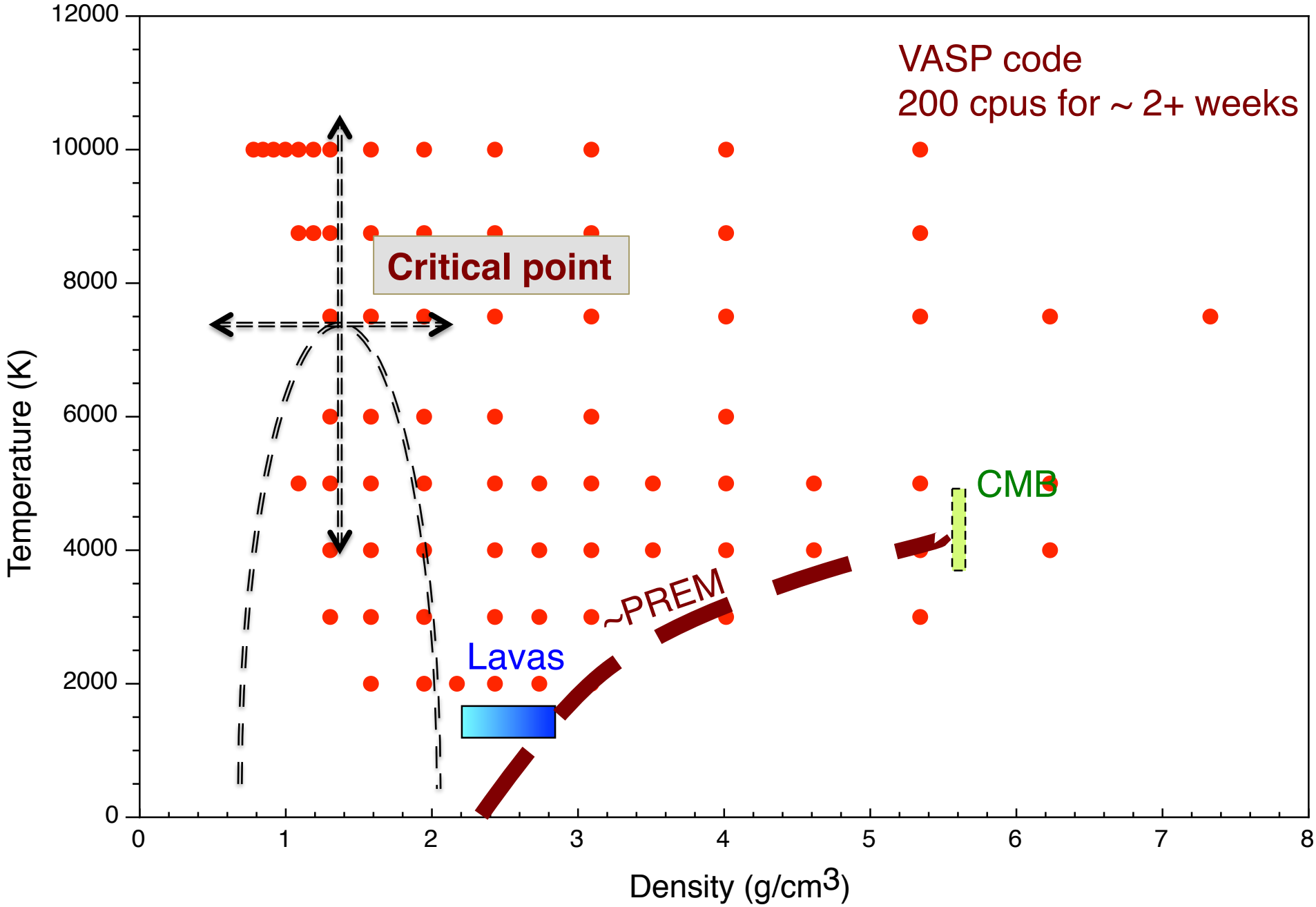

Temperature
Supercritical fluid
Liquid
Gas
Supercritical dome
Solid
Triple point
Density


Temperature
Density
Supercritical fluid
Supercritical point
Supercritical dome
Gas
Liquid
Solid
Triple point


12000
10000
8000
6000
4000
2000
0
Temperature (K)
0
1
2
3
4
5
6
7
8
Density (g/cm3)
Critical point
Magma Ocean ?
CMB
~PREM
Lavas


Pressure
Stable
vapor
Stable
liquid
LIQUID SPINODAL
reliable point from our simulations
Density


Super Critical temperature
SC
Critical point
V
L
L – V Equilibrium line
L – V Equilibrium line
L + V
Gas spinodal
Liquid spinodal
Pressure
Density

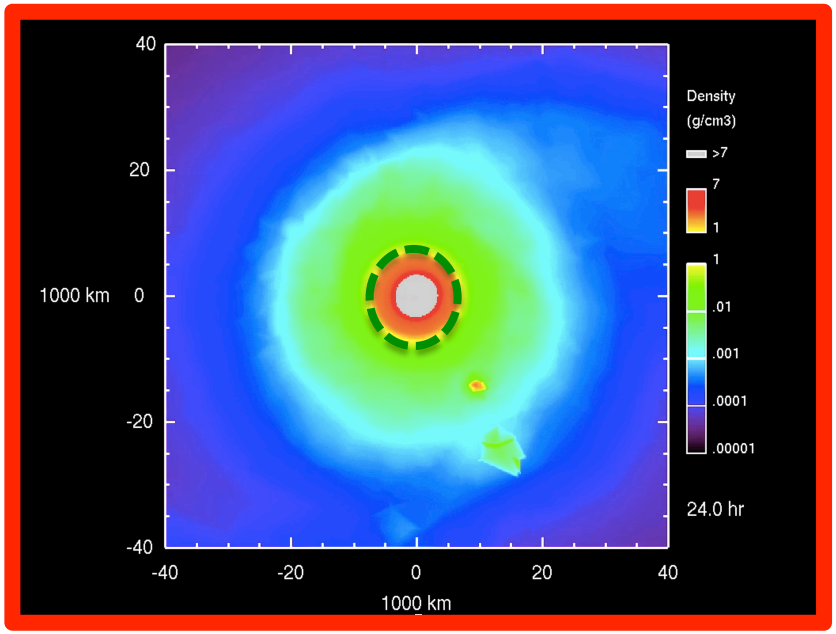

VASP code
200 cpus for ~ 2+ weeks
Critical point
CMB
~PREM
Lavas
Temperature (K)
Density (g/cm3)
12000
10000
8000
6000
4000
2000
0
0
1
2
3
4
5
6
7
8

C O N C L U S I O N S

Identifying the vapor vs liquid vs supercritical state is not trivial

- Bubbles nucleation spontaneous => marks the spinodal – the moment when the liquid becomes unstable
- This allows us to constrain the condensation of the protolunar disk
- The melt in supercritical state has peculiar properties, like speciation

CONCLUSIONS



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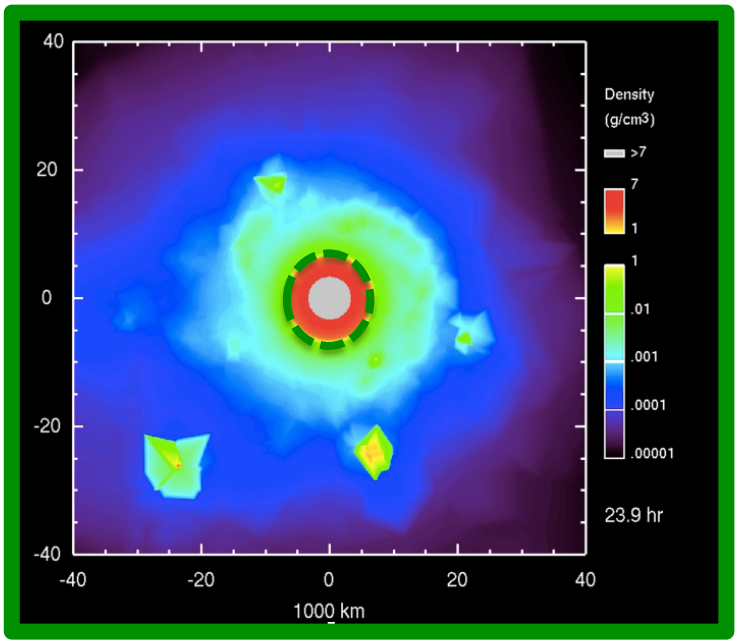

fast-spinning large proto-Earth + small impactor

Outer-green part:

- smaller than supercritical density => L + V
- volatiles and melt separate on cooling

Inner-green part:

- larger than supercritical density => L
- volatiles dissolved into melt, less degassing