AB INITIO PERSPECTIVE ON
GIANT IMPACTS AND PROTOLUNAR DISKS

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

https://moonimpact.eu/
I am in the basement at $10^{-15} \ldots -21$
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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
Every atom has a unique position and velocity.

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 \( (m) \).
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.
Update the position of every atom.

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 algorithms. 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.
Timesteps $\sim 1$ femtosecond
Statistics after $\sim$ ten(s) of picoseconds

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.
Density Functional Theory

ENERGY + CHARGE

ALL PHYSICAL PROPERTIES
We calculate the forces acting on the atoms.

From there we obtain velocities.

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

Čuk and Stewart, Science 2012
Density
Temperature
Solid
Gas
Supercritical fluid
Supercritical point
Supercritical dome
Liquid
Solid
Triple point
Density (g/cm$^3$)

Temperature (K)

Critical point

Lavas

~PREM

Magma Ocean ?

CMB

0

2000

4000

6000

8000

10000

12000

0

1

2

3

4

5

6

7

8
LIQUID SPINODAL
reliable point from our simulations

Stable vapor
Stable liquid
Pressure

Density

L

V

L + V

SC

Liquid spinodal

Gas spinodal

L – V Equilibrium line

Critical point

Super Critical temperature

L – V Equilibrium line

Liquid spinodal
Density (g/cm$^3$)

Temperature (K)

Critical point

~PREM

CMB

Lavas

VASP code
200 cpus for ~ 2+ weeks
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
similar sized impactor and proto-Earth

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