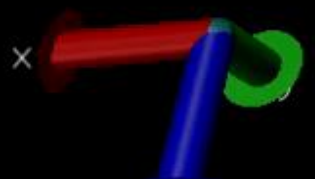
SIMULATING WATER ANALYZING DENSITY

ASELA CHANDRASINGHE



MOTIVATION

- Why study Molecular Dynamics?
- Why study water?

HOW DOES MD WORK?

- Langevin integrator
  - Like the Verlet method
  - Newtons equations of motion replaced with Langevin equations of motion

VERLET METHOD

Taylor expansion forward direction

$$y(t_i + \Delta t) = y(t_i) + \frac{dy}{dt}\Delta t + \frac{1}{2}\frac{d^2y}{d^2t}\Delta t^2 + \frac{1}{6}\frac{d^3y}{d^3t}\Delta t^3 + \ldots$$

Taylor expansion backward direction

$$y(t_i - \Delta t) = y(t_i) - \frac{dy}{dt}\Delta t + \frac{1}{2}\frac{d^2}{d^2t}\Delta t^2 - \frac{1}{6}\frac{d^3}{d^3t}\Delta t^3 + \ldots$$

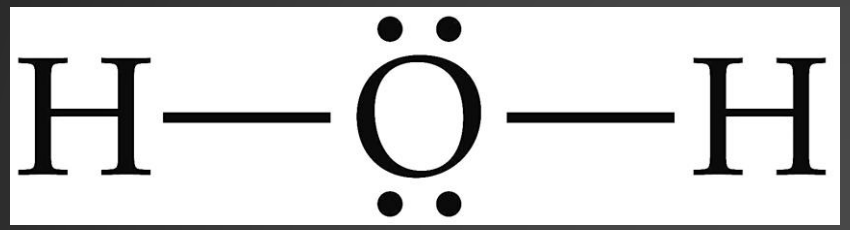
Forward + backward

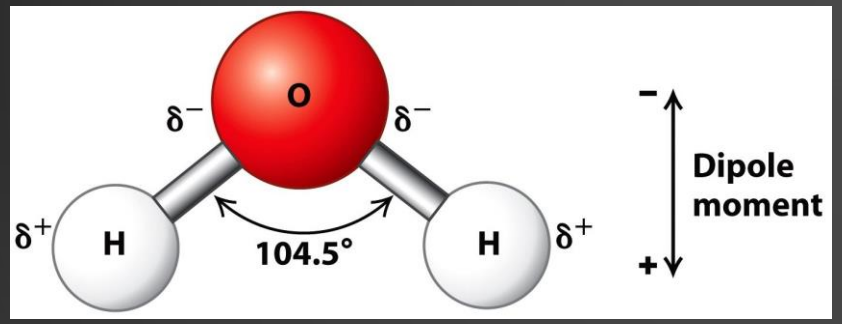
$$y_{i+1} = 2y_i - y_{i-1} + \frac{d^2y}{d^2t}(\Delta t^2)$$

FORCES (AMOEBA)

- Intermolecular
  - van der waal
  - dipole-dipole
  - charge- charge
  - quadrupole
- Intramolecular
  - bond stretching
  - bond bending

WATER STRUCTURE

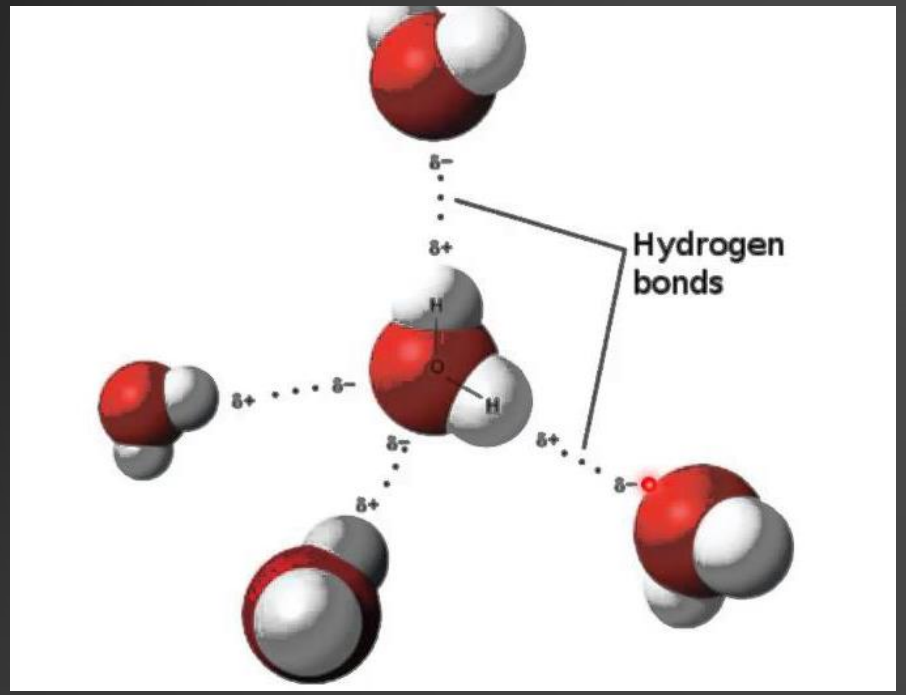




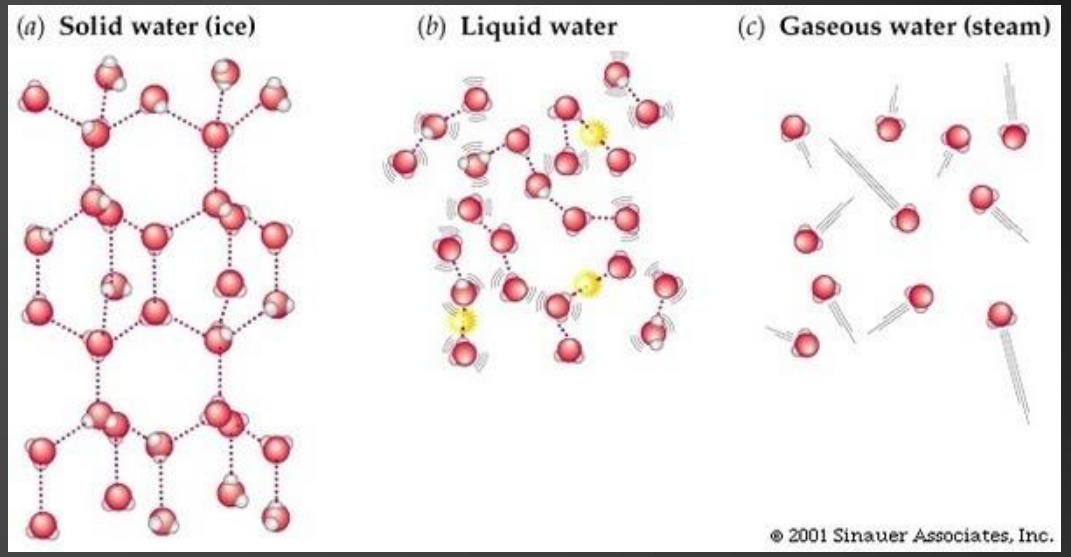
- 2 lone pairs
  - Bent geometry
- Covalent bonds
  - Partial charges
  - Hydrogen bonding

https://alevelbiology.co.uk/notes/water-structure-properties/
http://wt.kimiq.com/lewis-dot-diagram-for-water/

WATER PROPERTIES



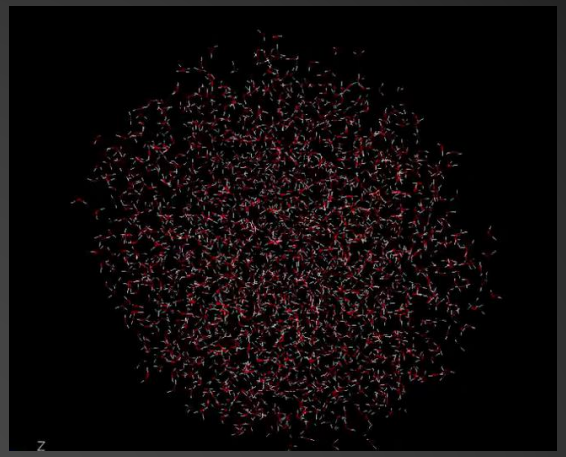
https://socratic.org/questions/how-is-hydrogen-bonding-among-water-molecules

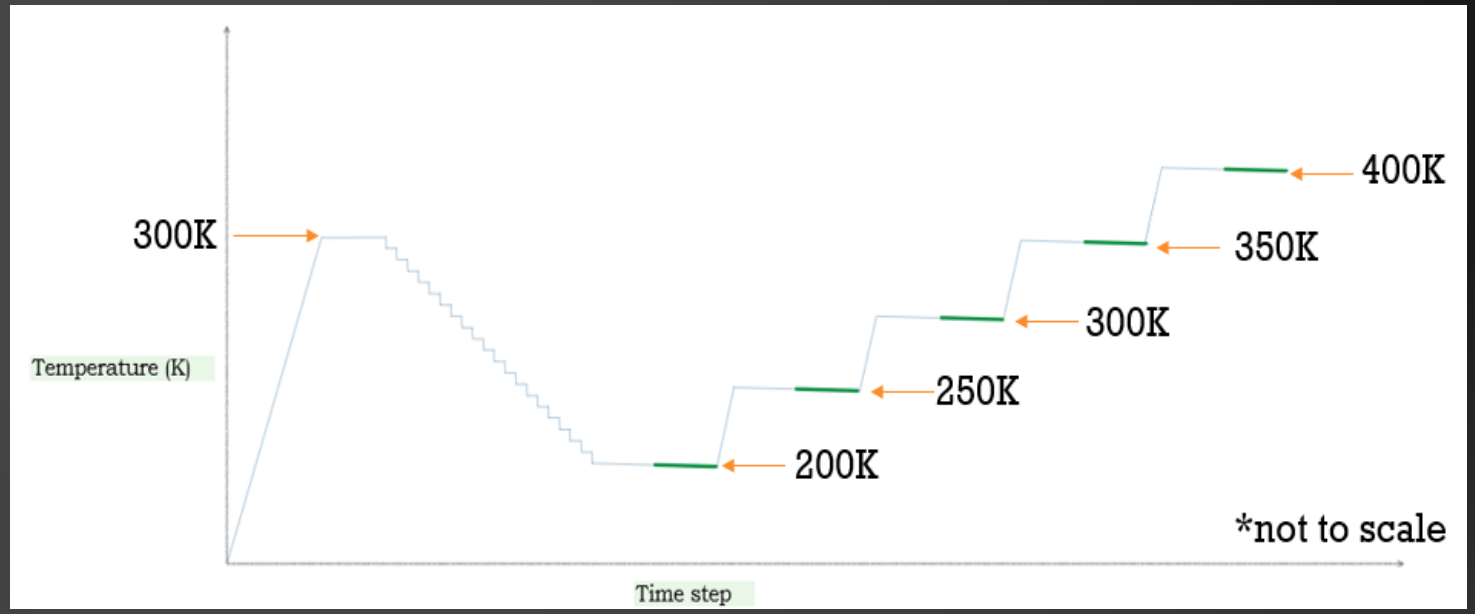


https://chem.libretexts.org/Textbook_Maps/General_Chemistry_Textbook_Maps

SIMULATION SETUP

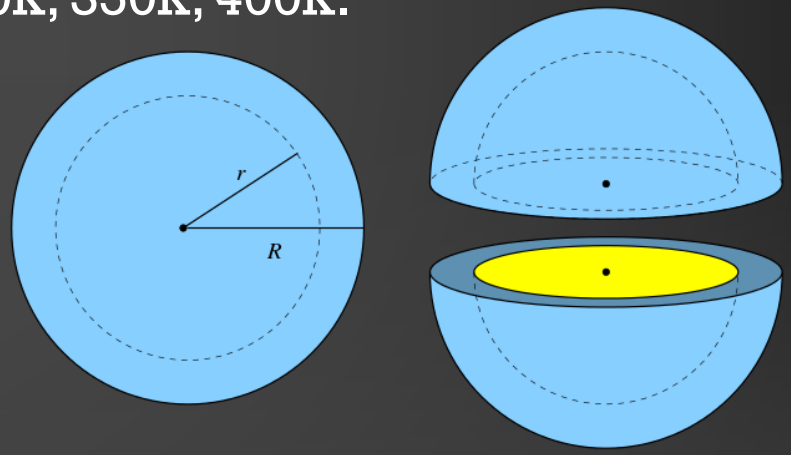
- 2,000 molecules
- Annealing in 11,500 time steps
  - 2,000 steps at 300K
  - 500 steps at each temp going down
- Equilibrate 1,000
- Collect every 40 steps for 4,000 steps (100 samples)





RESEARCH AIMS

- Density as a function of radius
- Rate of change in density with respect to radius
- Compare at temperatures of 200K, 250K, 300K, 350K, 400K.



NUMERICAL METHOD
NUMERICAL DERIVATIVE

Derivative Definition

$$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Numerical Derivative Applied

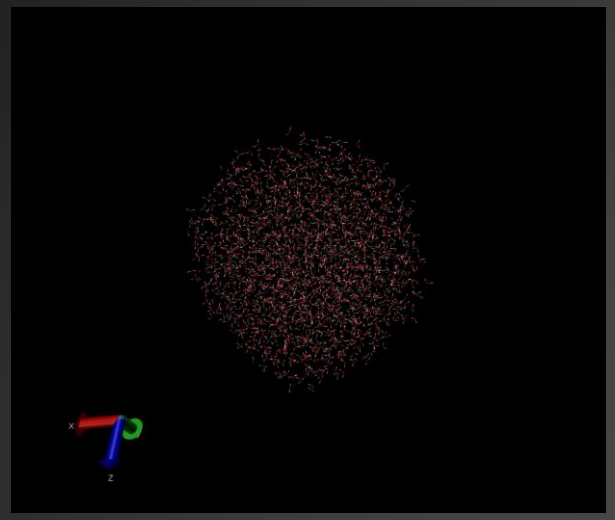
$$\frac{d\rho}{dr} \approx \frac{\rho(r+h) - \rho(r-h)}{2h}$$

Central Difference

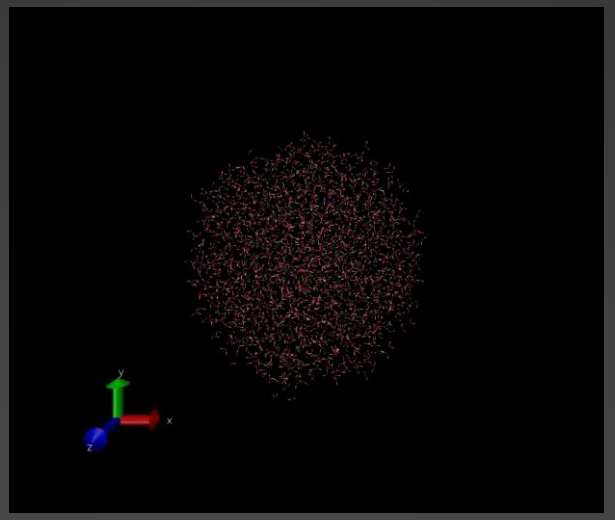
$$\frac{df}{dx} \approx \frac{f(x+h/2) - f(x-h/2)}{h}$$

$$\frac{d\rho}{dr} \approx \frac{\rho(r+h/2) - \rho(r-h/2)}{h}$$

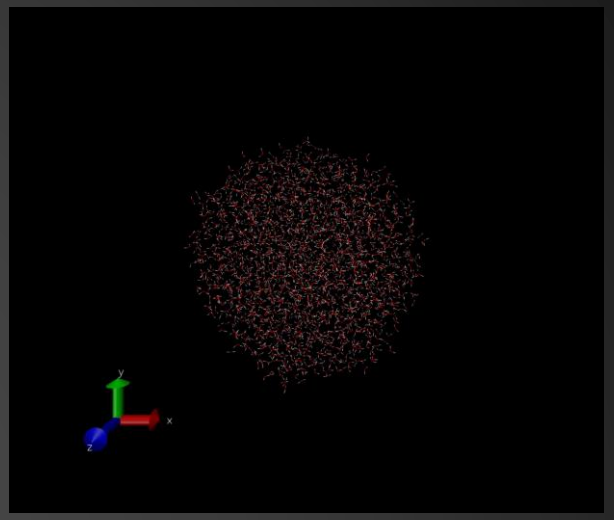
ρ = density
r = radius
h = width of spherical shell



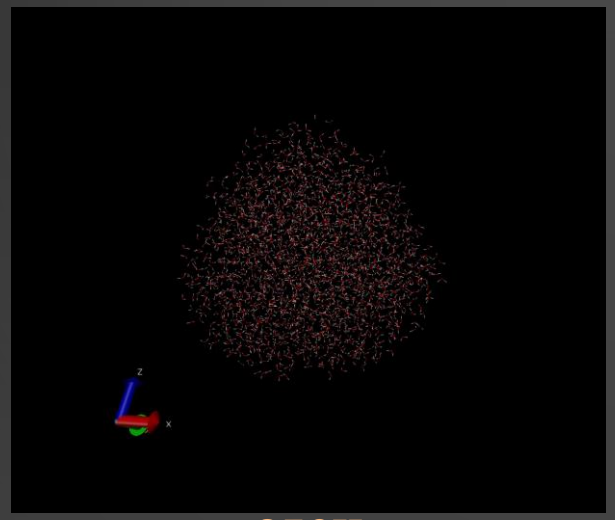
200K



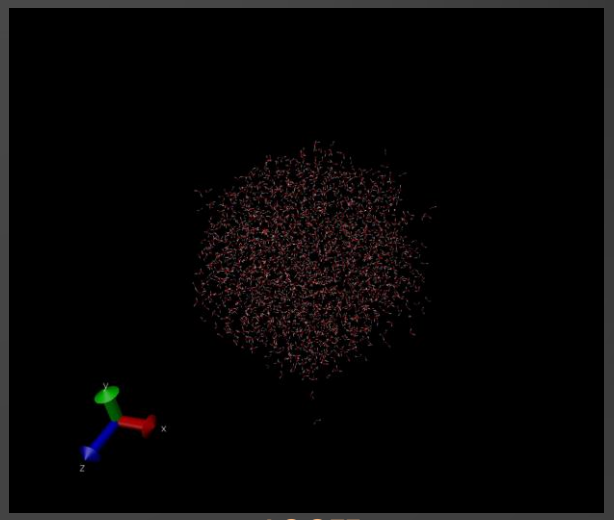
250K



300K

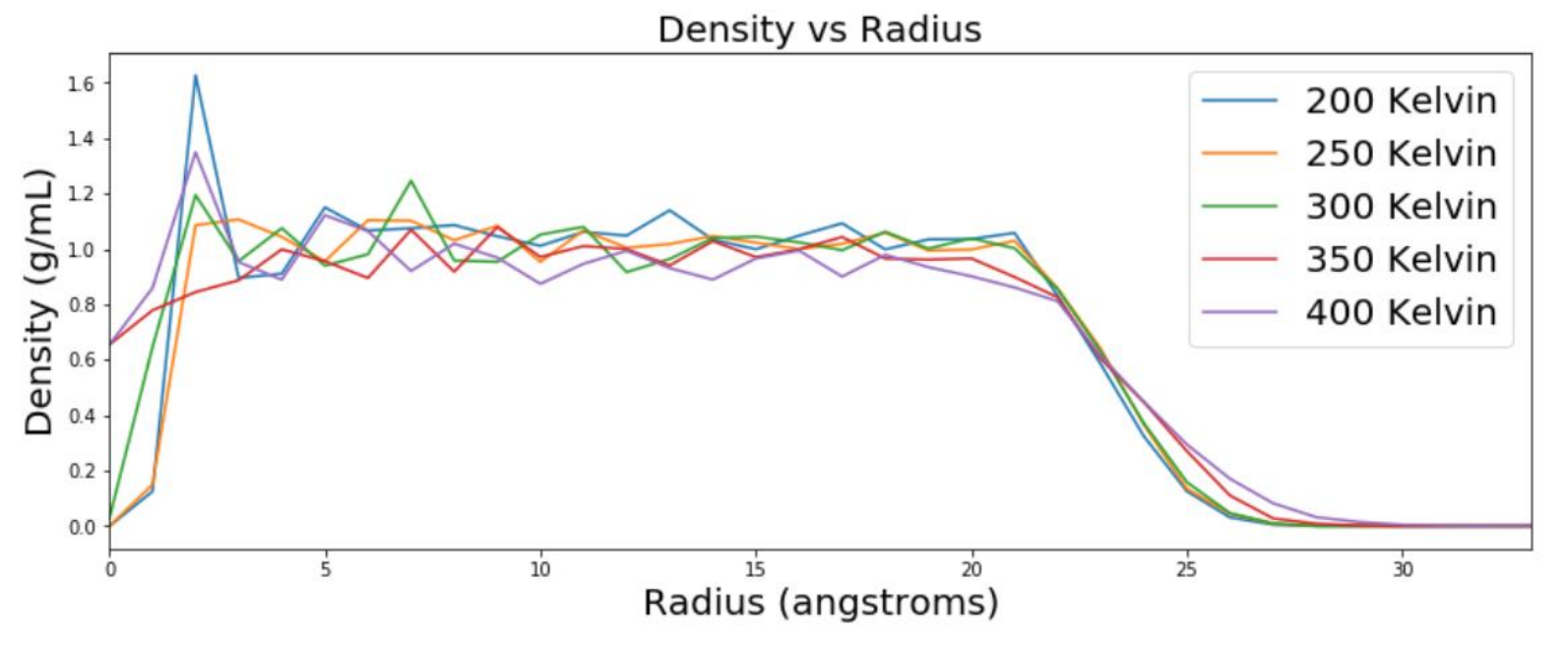


350K



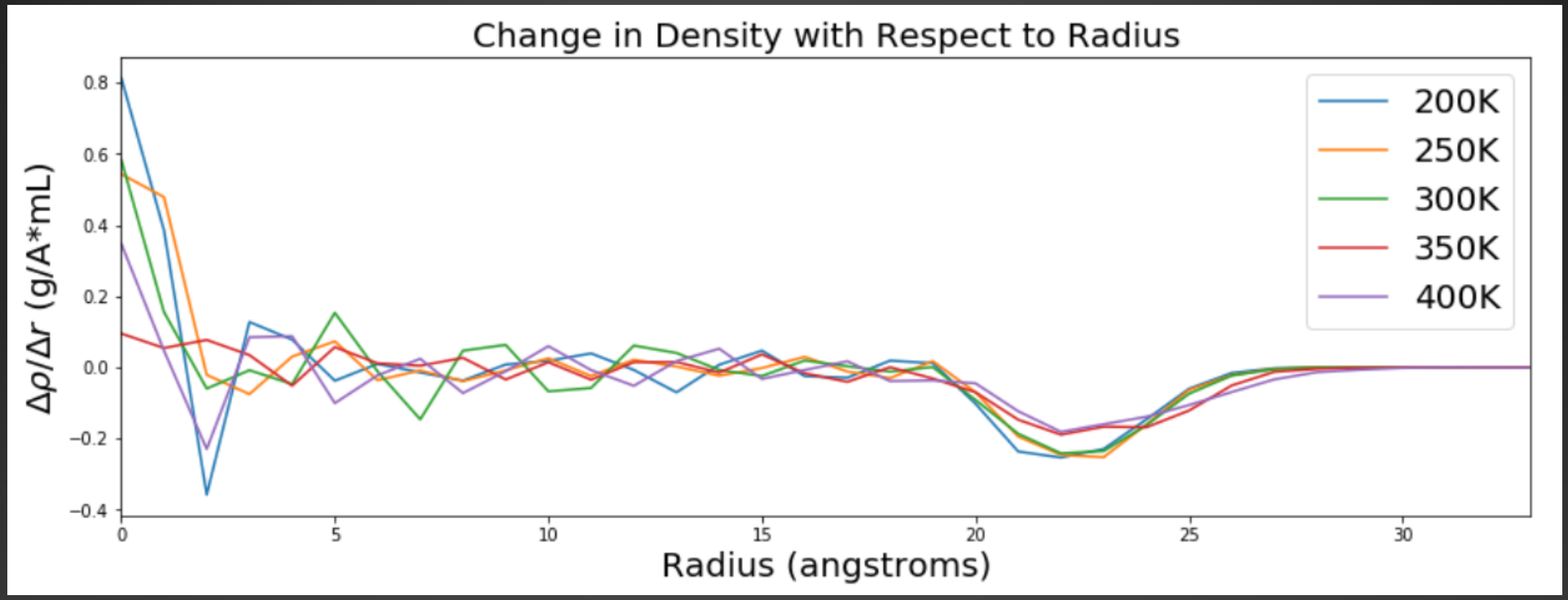
400K

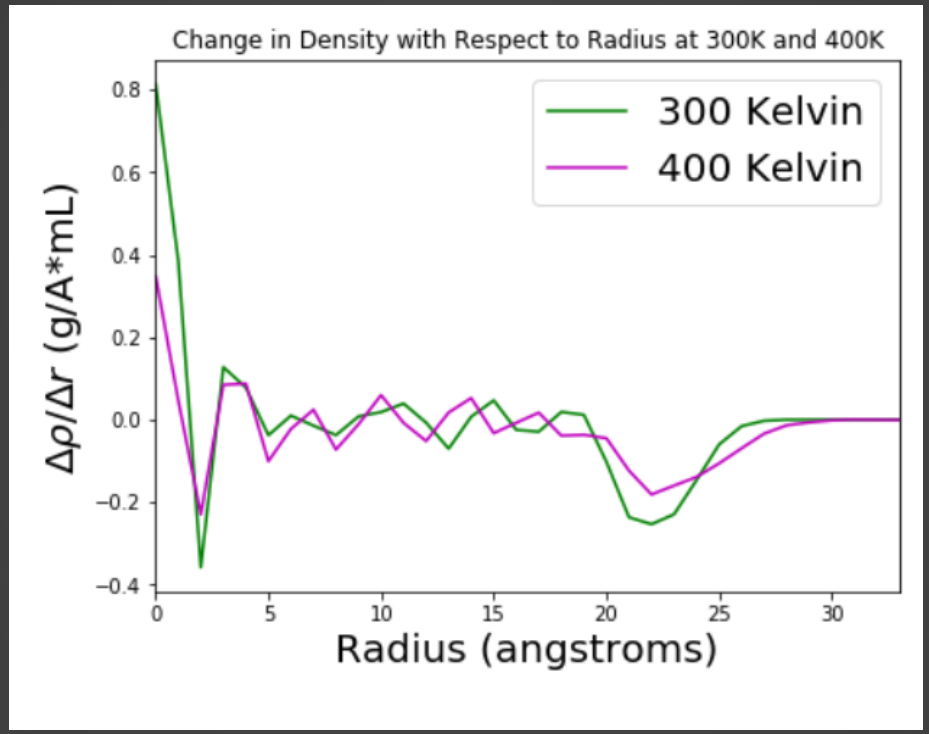
RESULTS



Temp (K)	Density (g/mL)
243 (solid)	0.983854
277 (liquid)	0.9999720
373 (boiling)	0.95835

Lide, D. R. CRC handbook of chemistry and physics. 12J204 2012.


Change in Density with Respect to Radius
Δρ/Δr (g/A*mL)
Radius (angstroms)
200K
250K
300K
350K
400K
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
0
5
10
15
20
25
30


Change in Density with Respect to Radius at 300K and 400K
300 Kelvin
400 Kelvin
Δρ/Δr (g/A*mL)
Radius (angstroms)
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
0
5
10
15
20
25
30

CONCLUSIONS

- In general water is behaving as expected
- For more detailed analysis simulations need to be altered

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