Thermal Simulations for the Scintillating Bubble Chamber Dark Matter Experiment

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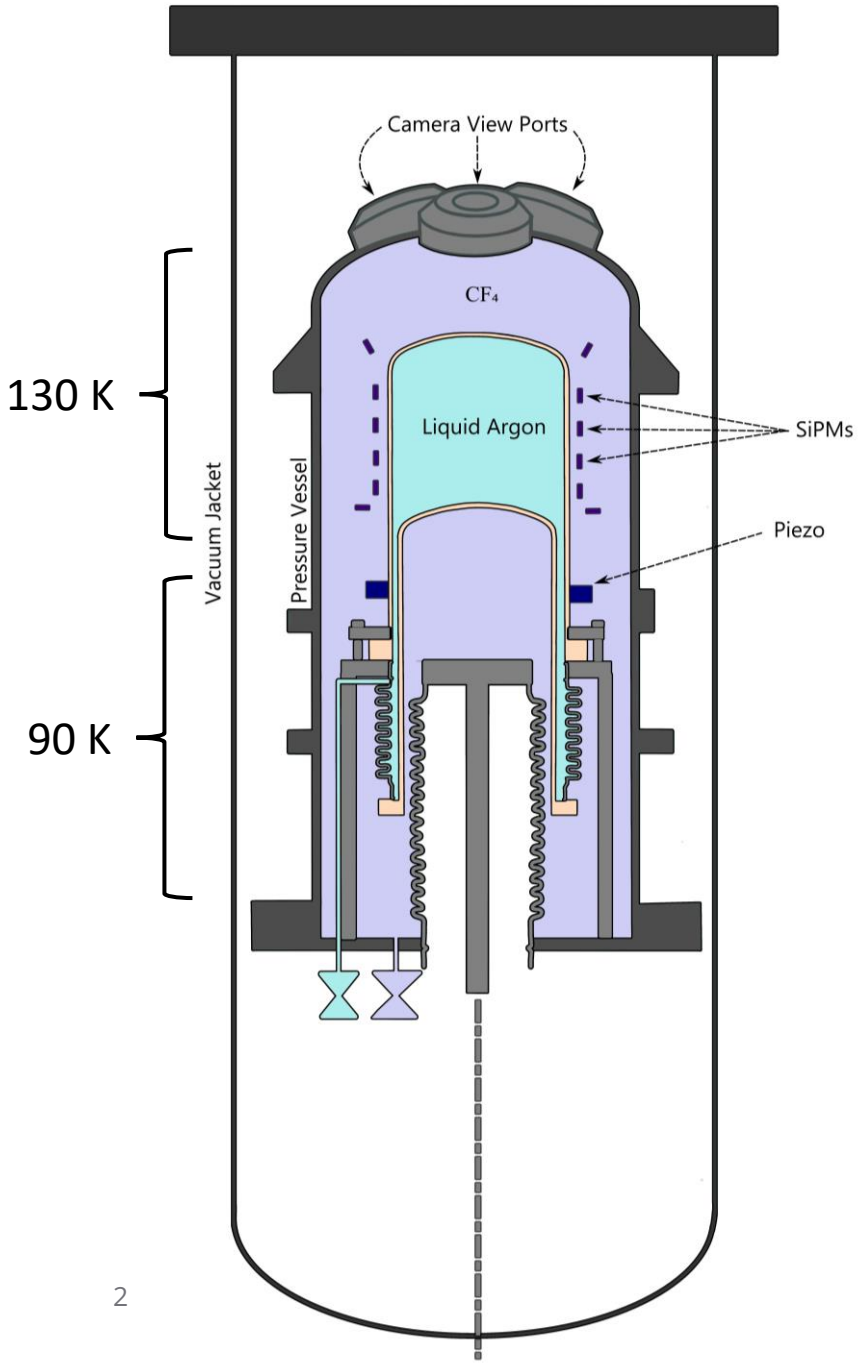
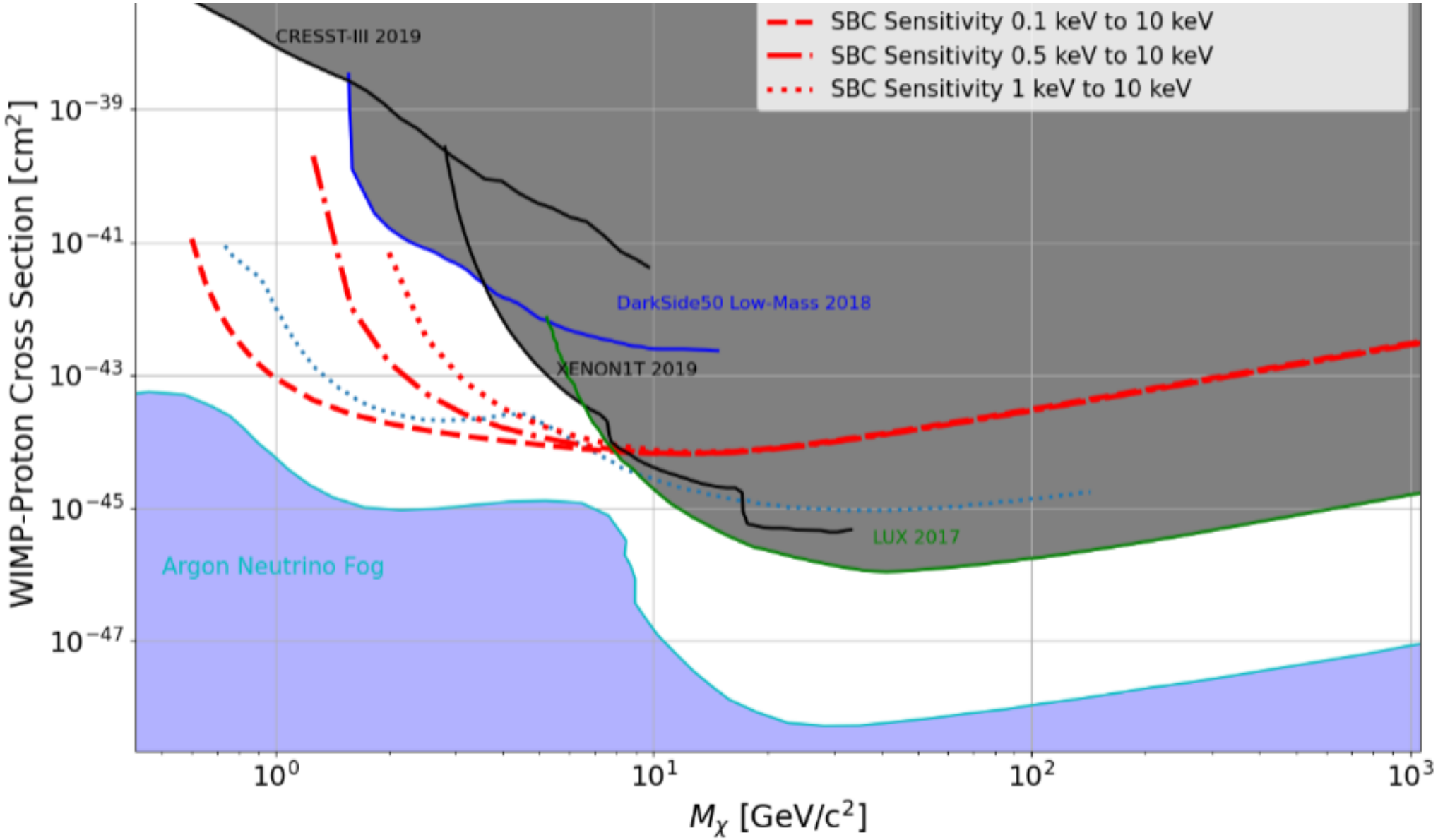


The Scintillating Bubble Chamber Detector

- Cryogenic liquid noble (Ar and Xe) bubble detectors
  - SBC-SNOLAB and SBC-LAr-10
- CF_4 Hydraulic Fluid
- Searching for low mass (< 10 GeV) dark matter
- Sensitivity to nuclear recoils down to 100 eV
- Scintillation allows for event-by-event energy reconstruction

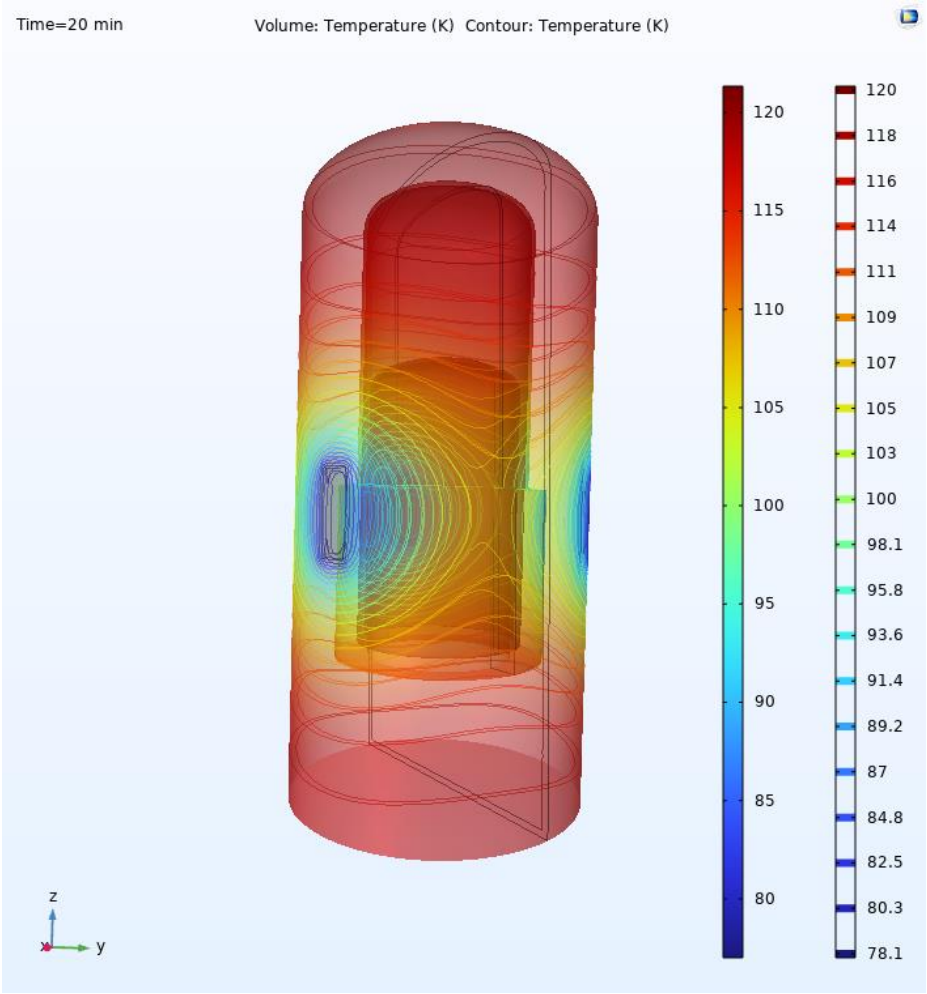


M. J. Bressler, PhD Thesis, 2022

Thermal Simulations

Bulk Fluid Simulations

- Modelling fluid flow in the detector
- Used for engineering design and operational tuning
- Limited by material properties available



Superheated Fluid

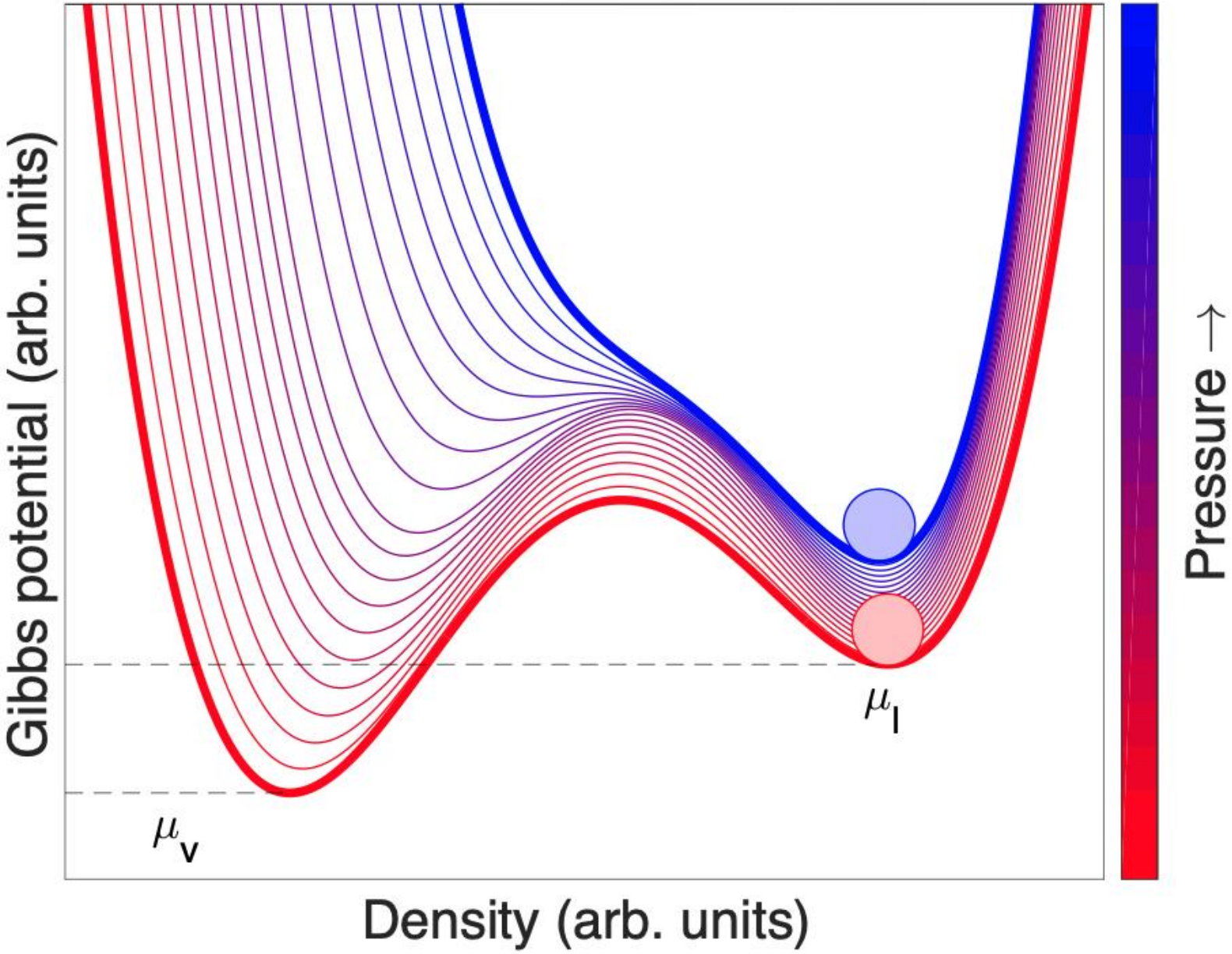
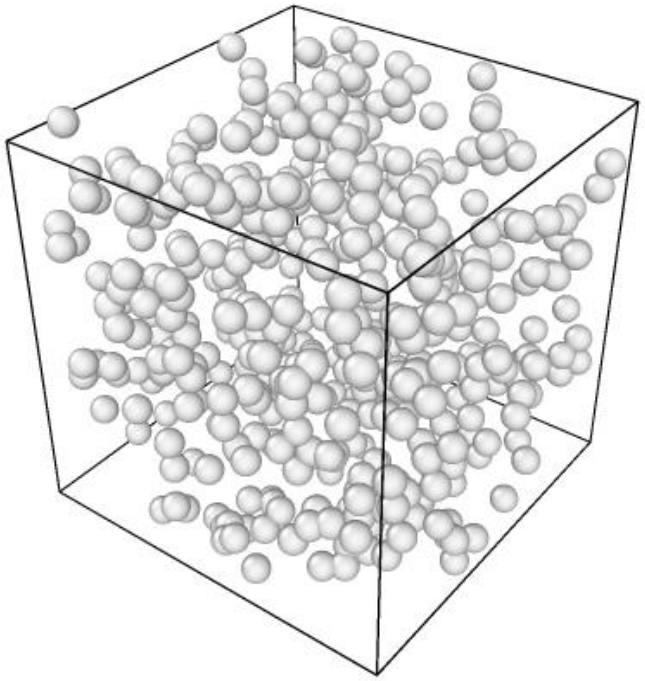


Image credit: Studio 52 Magic

Molecular Dynamics (MD) Simulations



- Lennard-Jones pair potentials → Bulk Properties
- Pair potential → Forces on each particle → Movement
- Multi-stage modelling approach

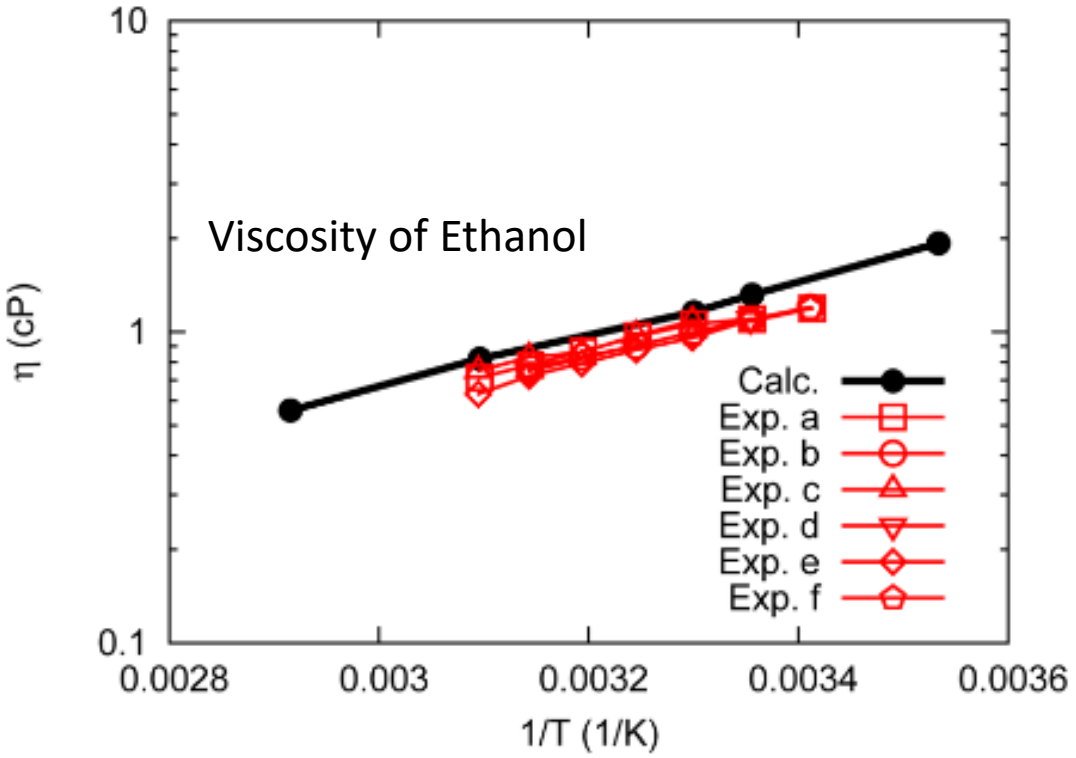
Green-Kubo Relations

- Relates random fluctuations at equilibrium to externally perturbed responses
- Allow for calculation of a transport coefficient based on the time correlation function of a corresponding “microscopic” variable
- Examples:
  - Viscosity from pressure tensors
  - Thermal conductivity from heat flow
  - Diffusion coefficient from velocity

$$\gamma = \int_0^\infty \langle \dot{A}(t)\dot{A}(0)\rangle \, \mathrm{dt}$$

$$\eta = \frac{\mathrm{V}}{k_b \mathrm{T}} \int_0^\infty \langle p_{\alpha\beta}(t) p_{\alpha\beta}(0)\rangle \mathrm{dt}$$

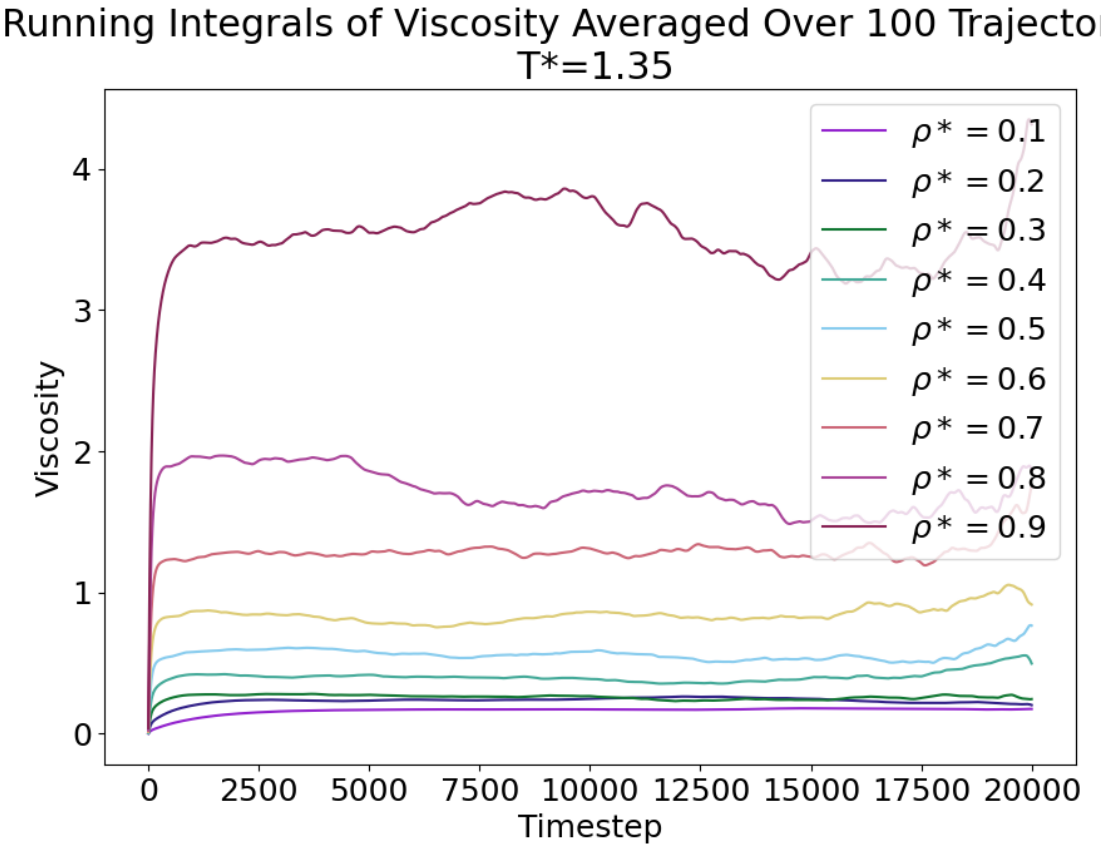
$$\kappa = \frac{\mathrm{V}}{k_b \mathrm{T}^2} \int_0^\infty \langle \mathrm{J}_\alpha(t)\mathrm{J}_\alpha(0)\rangle \, \mathrm{dt}$$

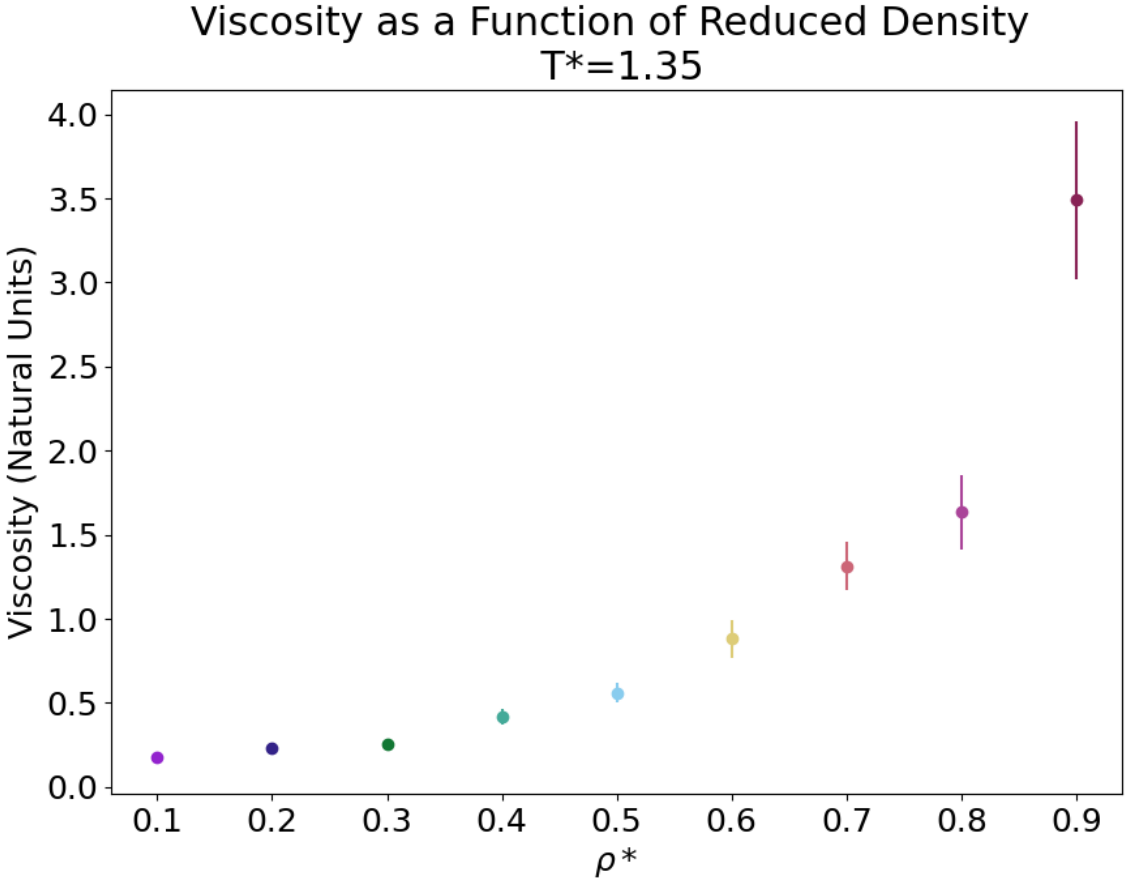


- Successful in other contexts to calculate:
  - Viscosity
  - Heat capacity
  - Thermal conductivity
  - Density
- Allows for calculation across a wide range of temperatures and pressures

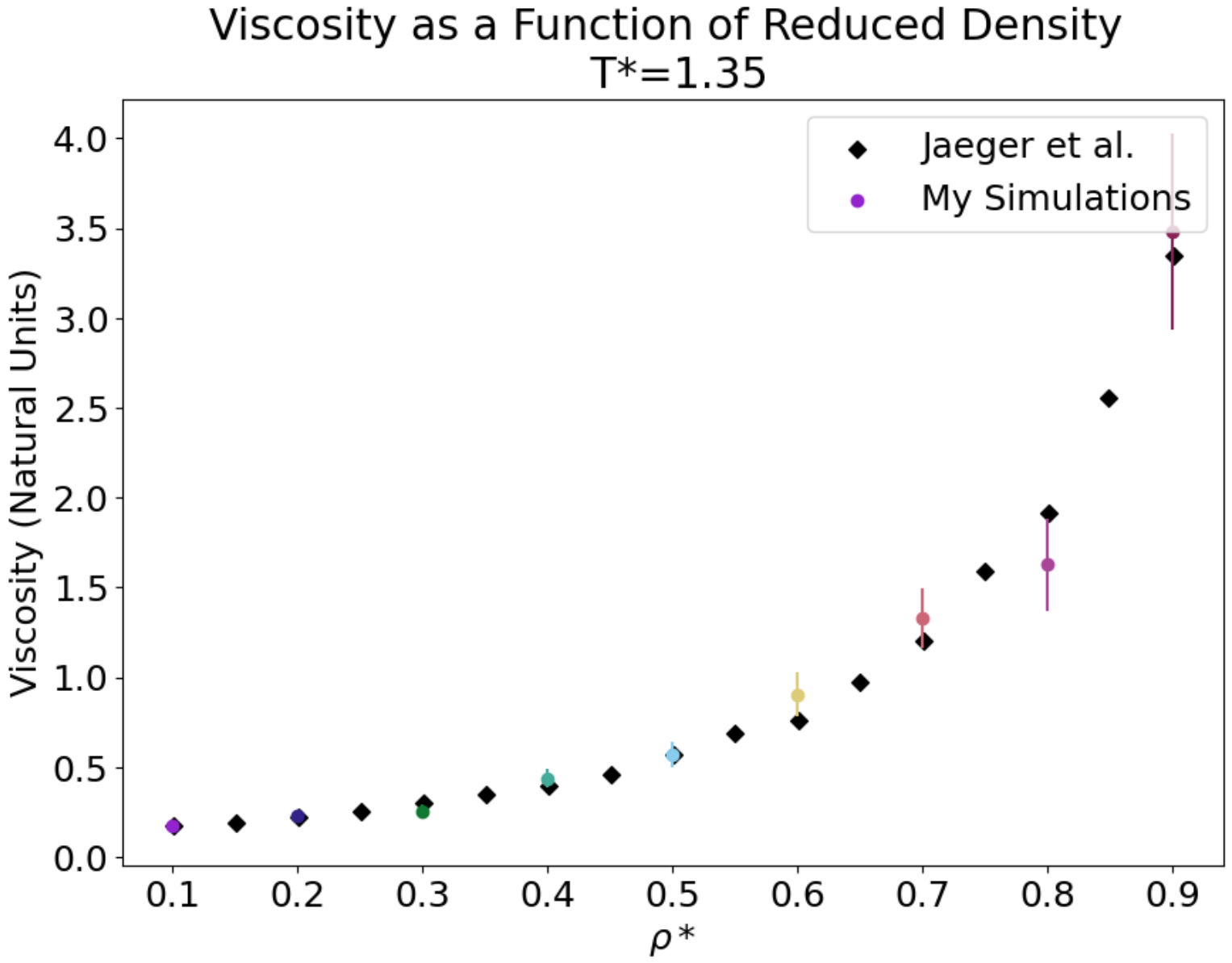
Reliable Viscosity Calculation from Equilibrium Molecular Dynamics Simulations: A Time Decomposition Method, Zhang, Y. ; Otani, A. ; Maginn, E. J.

Calculation of Viscosity in Natural Units



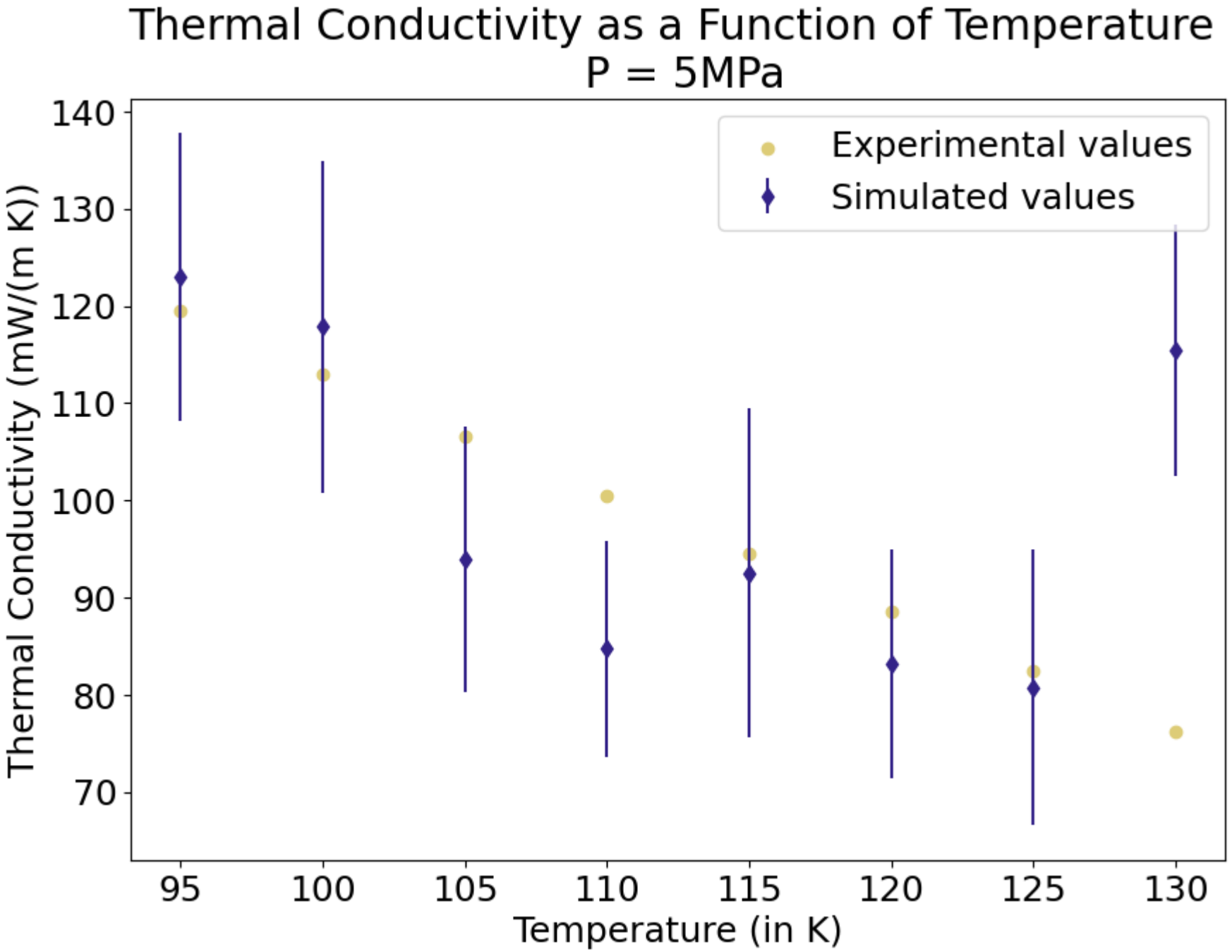


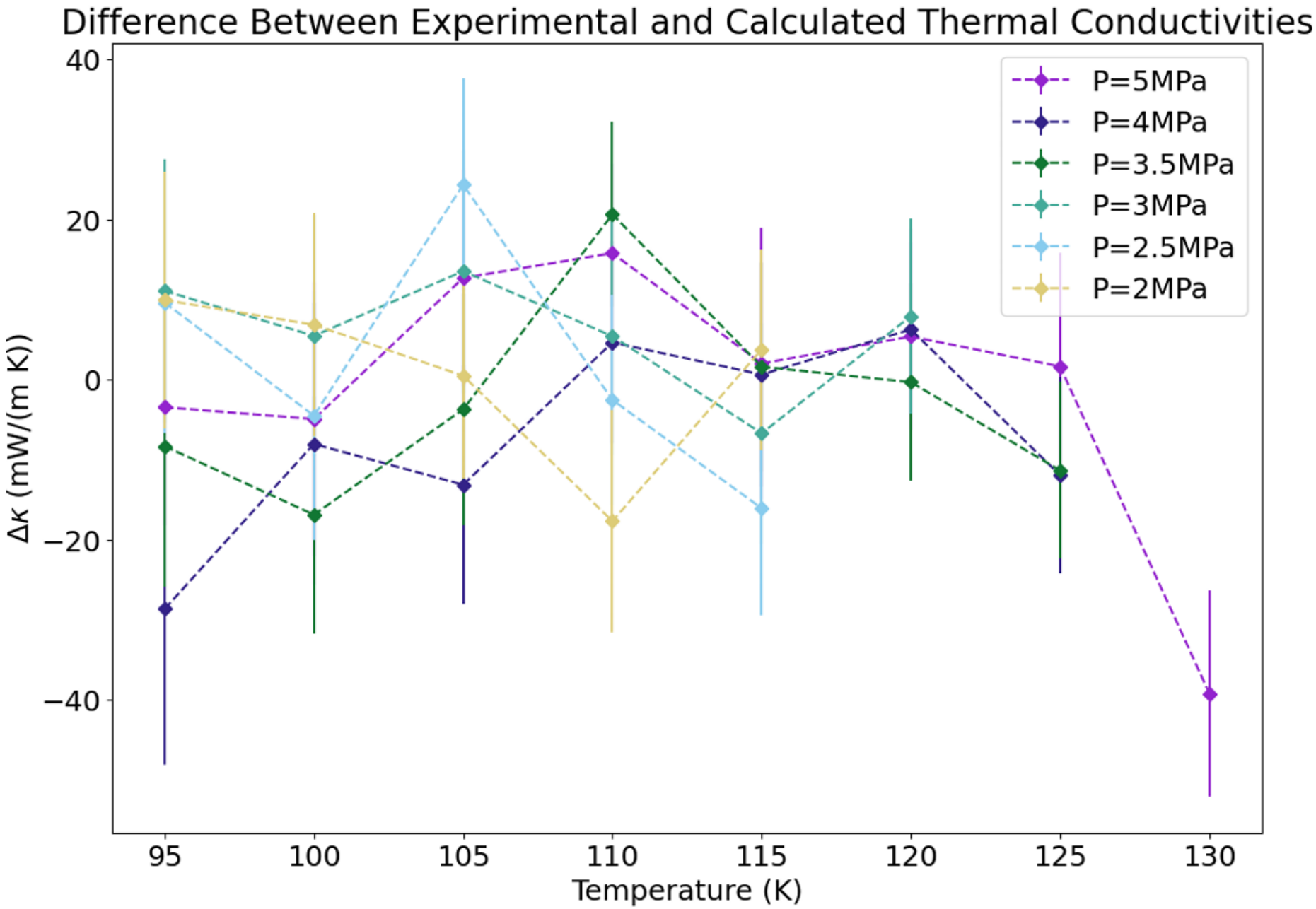
Comparison in Natural Units

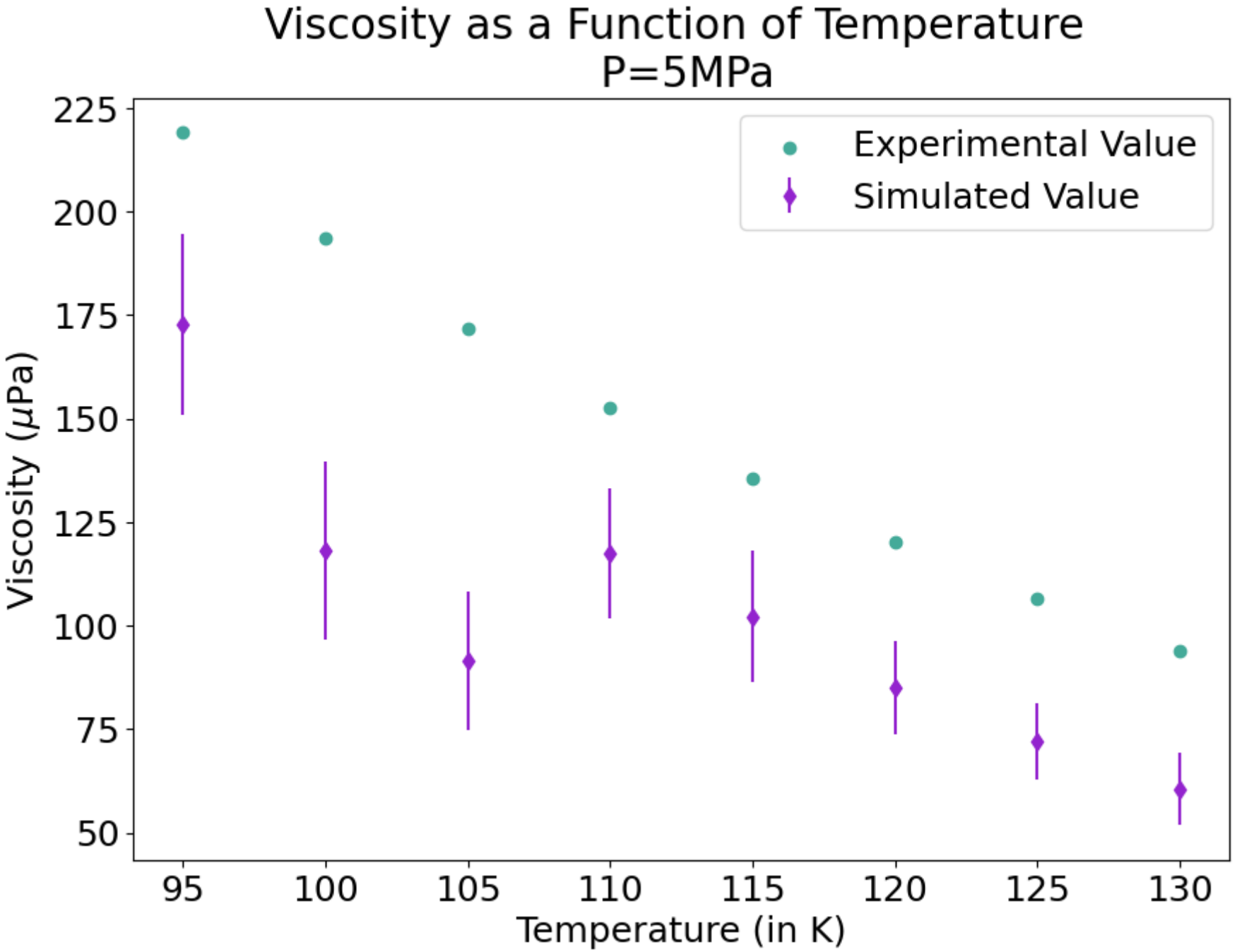


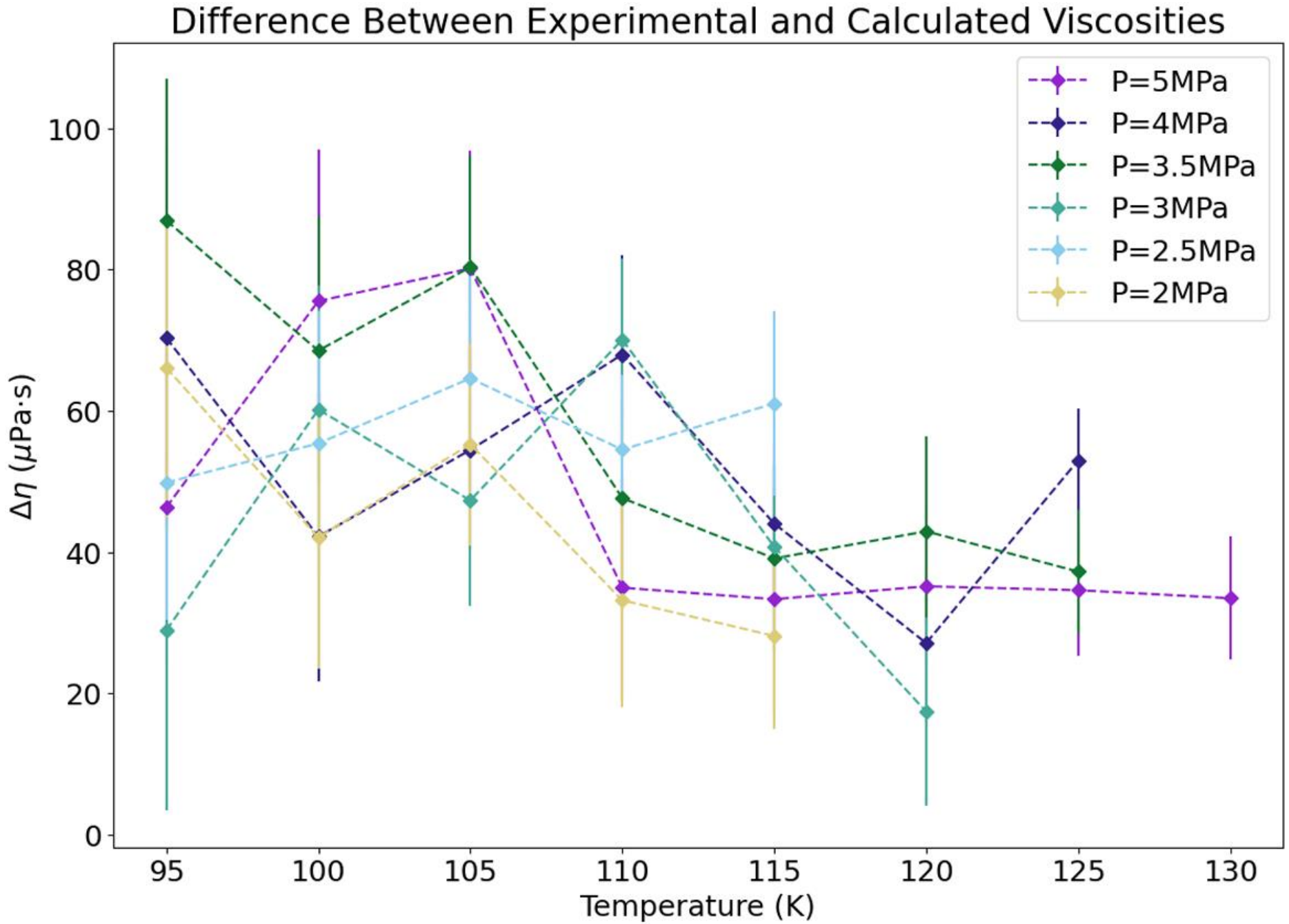
Black points from “Bulk Viscosity of Molecular Fluids” by Jaeger, Matar, and Müller.

Simulations of Liquid Argon



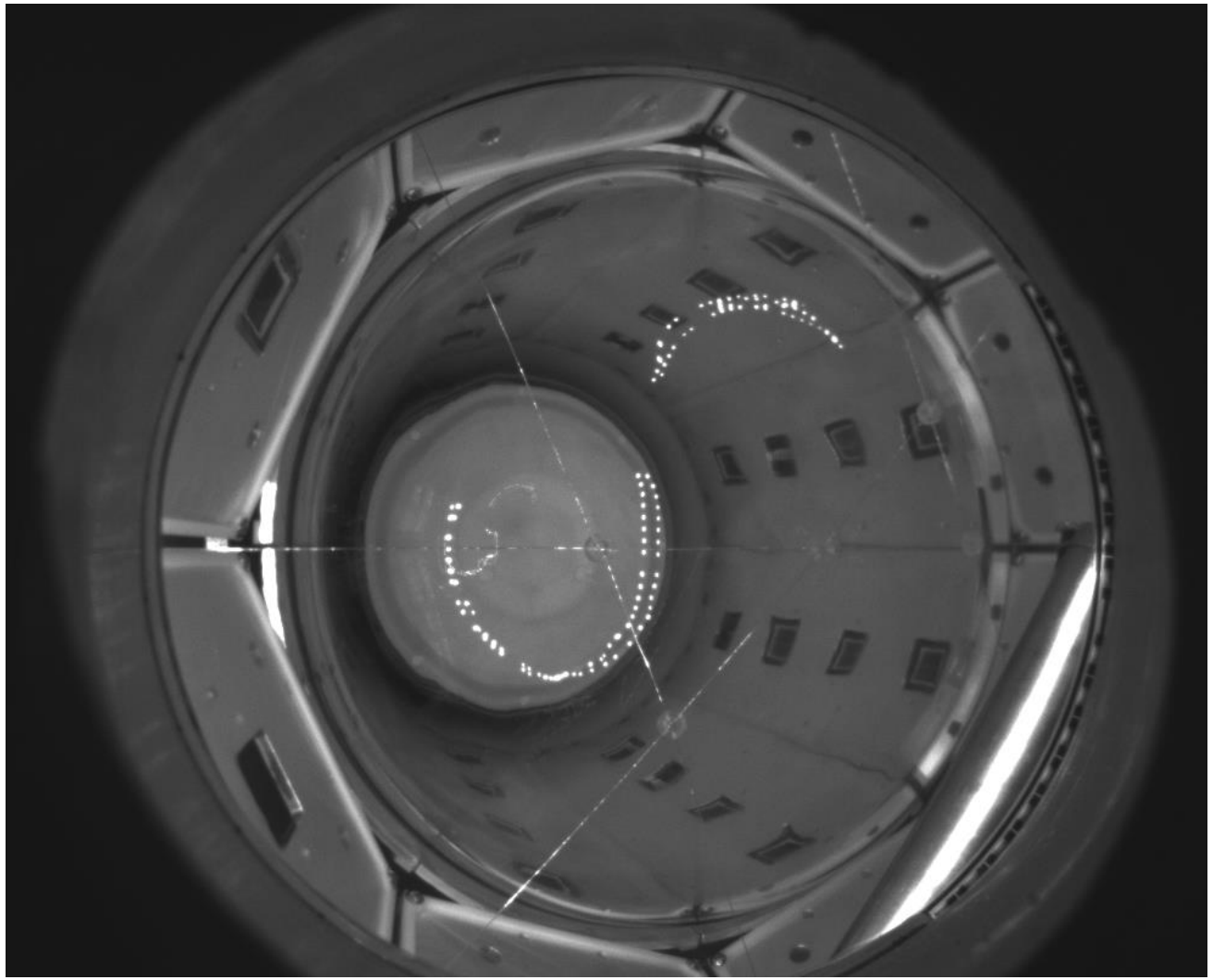

Difference Between Experimental and Calculated Thermal Conductivities
40
20
0
−20
−40
Δκ (mW/(m K))
95
100
105
110
115
120
125
130
Temperature (K)
P=5MPa
P=4MPa
P=3.5MPa
P=3MPa
P=2.5MPa
P=2MPa


Viscosity as a Function of Temperature
P=5MPa
Experimental Value
Simulated Value
Viscosity (μPa)
225
200
175
150
125
100
75
50
95
100
105
110
115
120
125
130
Temperature (in K)


Difference Between Experimental and Calculated Viscosities
P=5MPa
P=4MPa
P=3.5MPa
P=3MPa
P=2.5MPa
P=2MPa
Δη (μPa·s)
0
20
40
60
80
100
95
100
105
110
115
120
125
130
Temperature (K)

Future Work

- Extending approach to superheated argon
- Applying and comparing with CF_4
- Comprehensive study of how material choice affects success of this type of simulation
- Use of modified potentials to better reflect liquid behaviour, particularly for viscosity



Conclusions

Detection capability depends on strong thermal and fluid dynamic models:

- Nucleation threshold
- Two distinct temperature regions

Molecular dynamics → bulk fluid simulation framework

- Works well within some constraints

Lots of interesting future work!

Stay tuned for a thesis and a paper!