

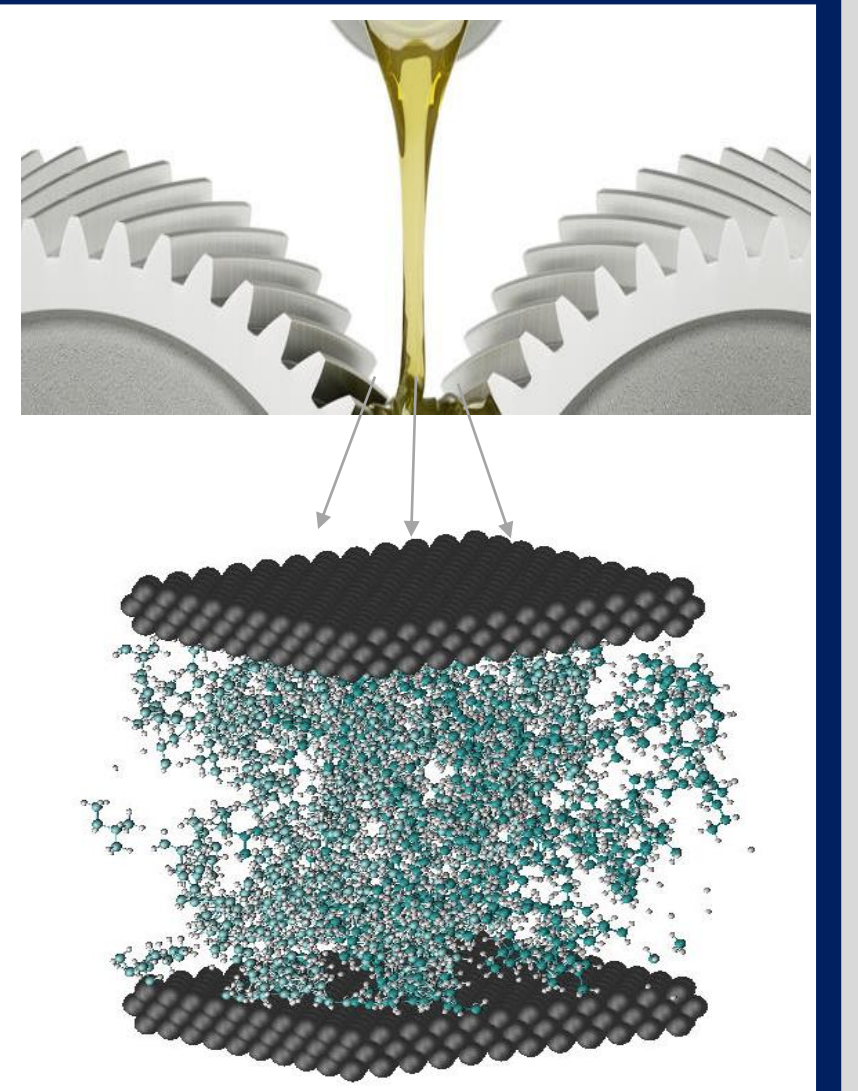
## Introduction

### Thermo-Elastohydrodynamic lubrication regime (TEHL)

- Very thin lubricant oil films (50 nm – 0,1 μm)
  - Extreme hydrodynamic pressure build-ups
  - High shear rates
  - High temperatures
- Difficult to characterize experimentally!
- Numerical modelling techniques needed  
→ **Molecular Dynamics (MD) simulations**

## Objectives

- Calculating lubricant properties under TEHL operating conditions using MD simulations
- Developing a reliable, accurate and robust methodology to extract these properties from MD



## Methodology

### MD simulations of lubricants

1. Equilibrium MD (EMD) → Newtonian behavior
2. Non-Equilibrium MD (NEMD) → Non-Newtonian behavior

#### EMD Methods

##### Green-Kubo

- Deals with autocorrelation functions (ACFs)
- Time integration of
  - stress tensor ACFs → Viscosity

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

##### Einstein

- Deals with mean-squared displacements (MSDs)
- At large  $t$ , linear relation between  $t$  and MSD of stress tensor → viscosity

$$\eta = \lim_{t \rightarrow \infty} \frac{1}{2} \frac{V}{k_B T} \langle (P_{\alpha\beta}(t) - P_{\alpha\beta}(0))^2 \rangle$$

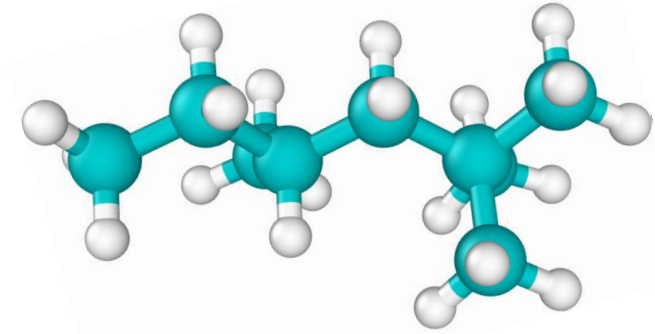
Accuracy of EMD = interaction potentials  
+ **post-processing methodology**

Post-processing EMD with Green-Kubo & Einstein formulations:

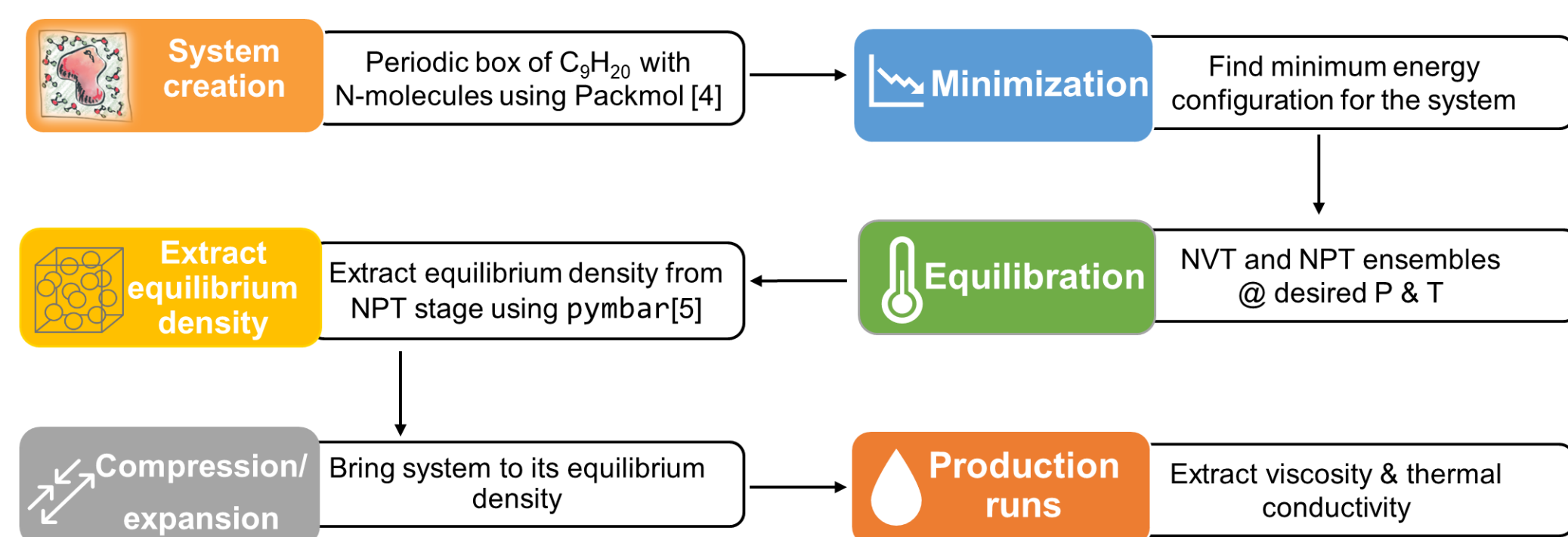
- **ad-hoc technical parameters/settings** → heavily affects the results → no standard procedure!
- Reliable extraction of lubricant properties from EMD
  - ❑ Improved statistics/robustness by averaging over short multiple independent trajectories
  - ❑ Automatically determining the region from which the property of interest extracted
  - ❑ Calculating uncertainty on the lubricant properties

## Results

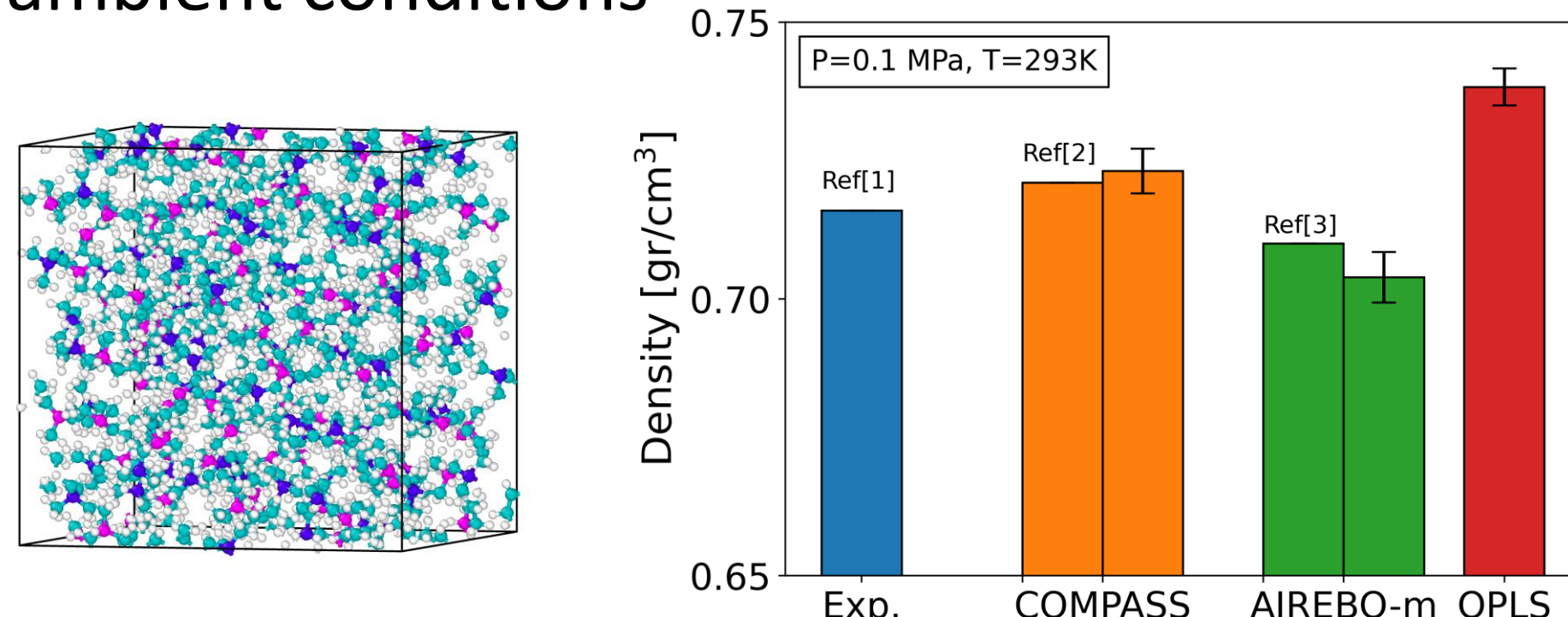
- 2,2,4-trimethylhexane molecule,  $C_9H_{20}$



- MD protocol:

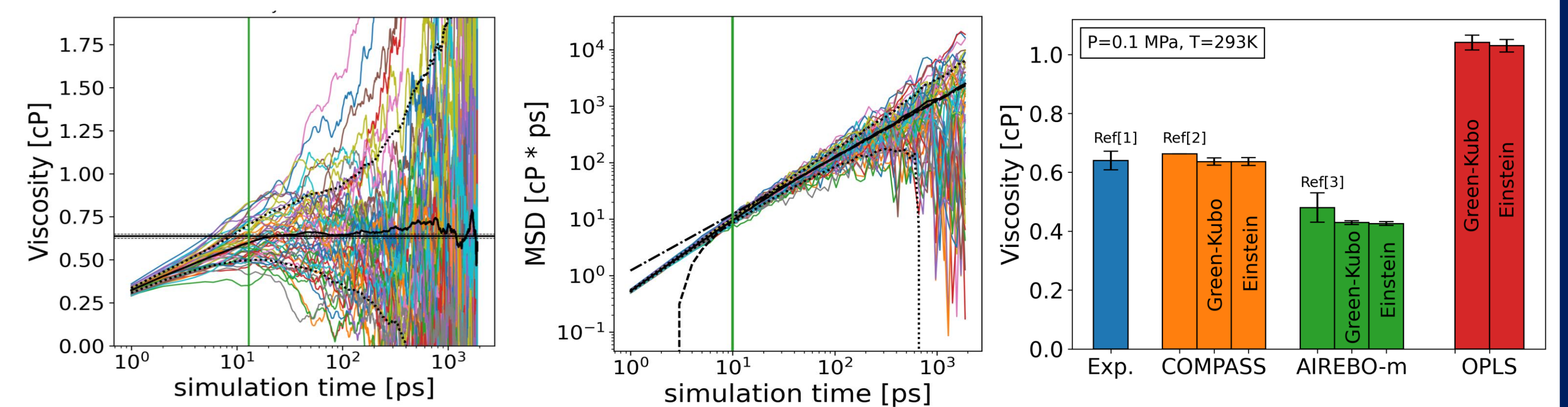


- 3 different interaction models (COMPASS, OPLS, AIREBO-m) under ambient conditions



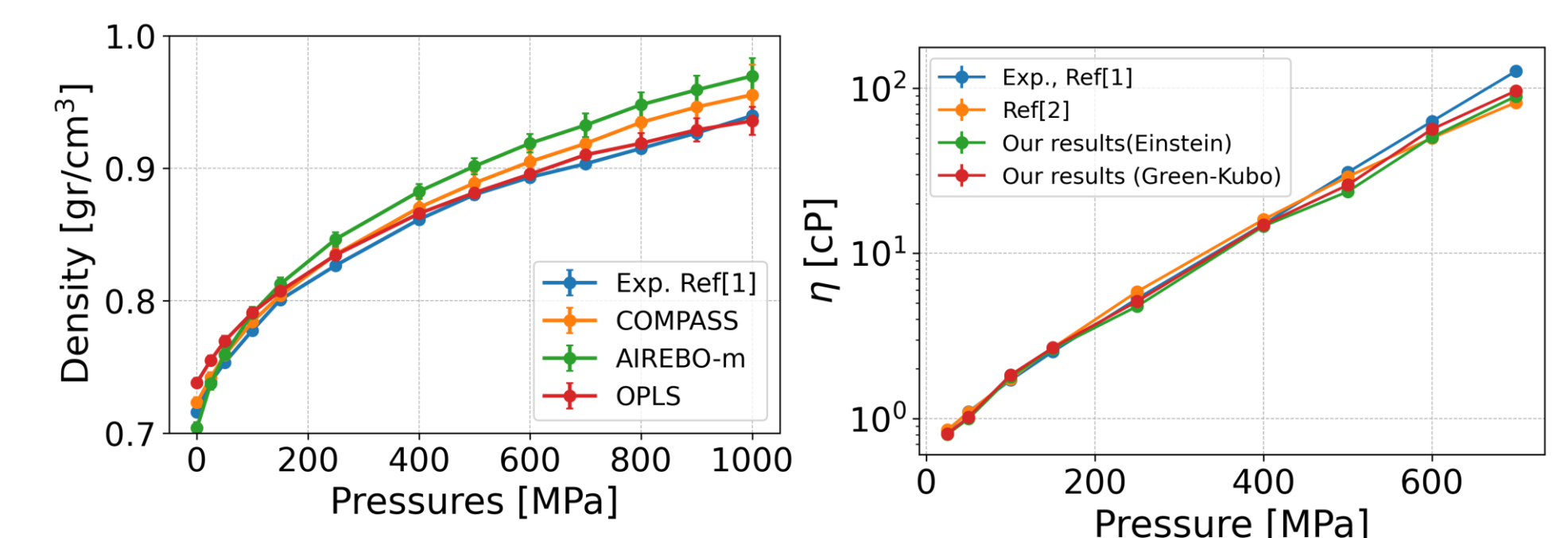
\*All the simulations were performed using the LAMMPS MD code [6]

- Viscosity calculated as an average from 50 independent production runs

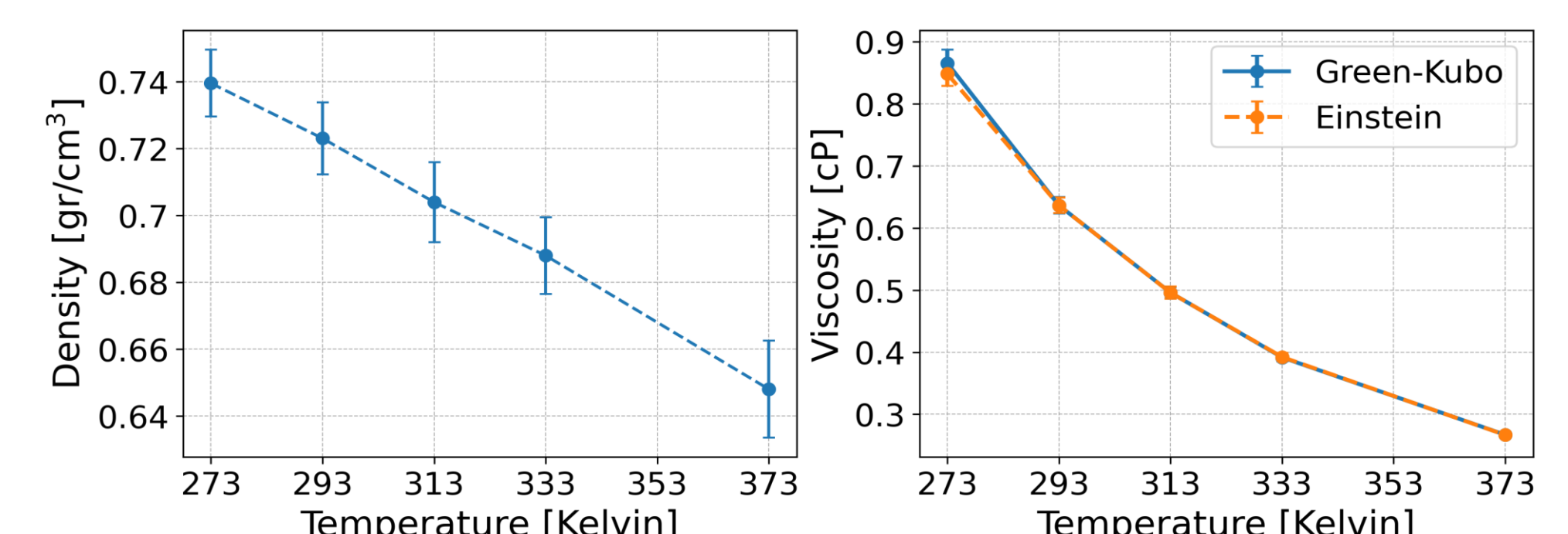


- Density & viscosity dependence on pressure & temperature with COMPASS

#### Pressure



#### Temperature



## Conclusions

- A post-processing methodology with improved accuracy/robustness and reliability
- Most accurate estimations of density and viscosity under ambient conditions with COMPASS FF
- Accurate estimation of density up to 1 GPa pressure with all FFs
- Under-estimation of viscosity above 400 MPa
  - EMD methods computationally very expensive at high pressures due to increased decay time constants of molecules
- Accurate estimation of density & viscosity at temperature

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