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Simulation-Based Phase Diagram Construction for van der Waals Fluids

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Phase separation underlies the formation of biomolecular condensates such as stress granules and nucleoli. Constructing a temperature–density-dependent phase diagram is essential for identifying the conditions that enable their formation. To this end, we investigated van der Waals fluids using molecular dynamics simulations and developed different complementary approaches: based on clustering analysis, and on thermodynamic observables such as specific heat and surface tension.
By applying the SPACEBALL algorithm to calculate cluster volumes and densities, we extracted binodal and spinodal lines across a wide range of temperatures and densities. Our results yield a consistent critical temperature ($T^* \approx 1.31$) and show strong agreement with theoretical expectations.
These methods offer a practical framework for mapping phase behavior in systems lacking a defined equation of state, providing valuable tools for studying liquid-liquid phase separation in protein solutions, including those associated with neurodegenerative diseases.

References

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