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Can we better use existing and emerging computing hardware to embed activity coefficient predictions in complex atmospheric aerosol models?

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To predict the evolving concentration, chemical composition and ability of aerosol particles to act as cloud droplets, we rely on numerical modeling. Mechanistic models attempt to account for the movement of compounds between the gaseous and condensed phases at a molecular level. This 'bottom up' approach is designed to increase our fundamental understanding. However, such models rely on predicting the properties of molecules and subsequent mixtures. For partitioning between the gaseous and condensed phases this includes: saturation vapour pressures; Henrys law coefficients; activity coefficients; diffusion coefficients and reaction rates. Current gas phase chemical mechanisms predict the existence of potentially millions of individual species. Within a dynamic ensemble model, this can often be used as justification for neglecting computationally expensive process descriptions. Indeed, on whether we can quantify the true sensitivity to uncertainties in molecular properties, even at the single aerosol particle level it has been impossible to embed fully coupled representations of process level knowledge with all possible compounds, typically relying on heavily parameterised descriptions.

Relying on emerging numerical frameworks, and designed for the changing landscape of high-performance computing (HPC), in this study we show that comprehensive microphysical models from single particle to larger scales can be developed to encompass a complete state-of-the-art knowledge of aerosol chemical and process diversity. We focus specifically on the ability to capture activity coefficients in liquid solutions using the UNIFAC method, profiling traditional coding strategies and those that exploit emerging hardware.