

# Kirkwood-Buff integrals from molecular simulation

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The Kirkwood-Buff (KB) theory provides a rigorous framework to predict thermodynamic properties of isotropic liquids from the microscopic structure [1, 2]. Several thermodynamic quantities relate to KB integrals, such as partial molar volumes. KB integrals are expressed as integrals of Radial Distribution Functions (RDF) over volume but can also be obtained from density fluctuations in the grand-canonical ensemble [3]. Various methods have been proposed to estimate KB integrals from molecular simulation. In this presentation, based on reference [4], I will review the available methods to compute KB integrals from molecular simulations of finite systems, and particular attention will be paid to finite-size effects [4, 5]. I will also review various applications of KB integrals computed from simulations. These applications demonstrate the importance of computing KB integrals for relating findings of molecular simulation to macroscopic thermodynamic properties of isotropic liquids.

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