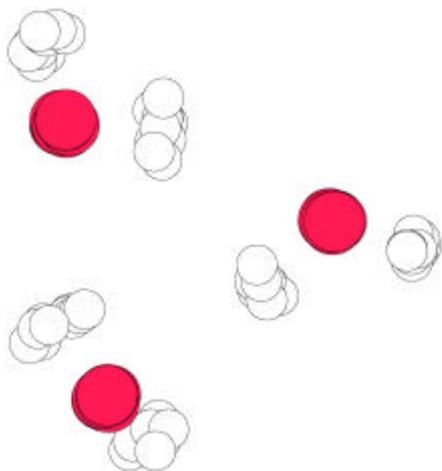


A study of massively parallel implementations of quantum statistical mechanics algorithms

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The quantum mechanics of electrons determines the nature of the chemical bond. The quantum mechanics of molecular nuclei determine the nature of detailed interactions between molecules. The development of techniques based on quantum statistical mechanics are necessary to accurately predict the thermodynamics of molecular species from first principles. We have initiated a study of Monte Carlo Feynman path integration simulation techniques on massively parallel architectures, in an effort to accurately calculate thermodynamic properties.