**Free energy calculations and polarisable force fields**

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The use of the LAMMPS USER-FEP package for free energy calculations using perturbation and related techniques will be presented with examples of determination of free energies of solvation. The calculation of potentials of mean force using umbrella sampling will also be illustrated. An important evolution in classic force fields is the incorporation of explicit polarisation (induction) to represent the response of election clouds to the electrostatic environment. The QEQ and USER-DRUDE packages, which implement fluctuating charges and induced dipoles, will be presented.