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| Session title: | | Grand Canonical ensemble and detailed balance | | | Course: MC2001 |
| Aims: | | Introduce grand canonical ensembles: outline, uses and additional move types.  Demonstrate the use of GCMC on a model system and assess how various parameters affect the outcome of the simulation. | | | |
| Intended learning outcomes (ILOs) : | | | 1. Define the Grand Canonical (GC) ensemble 2. Outline some uses for the Grand canonical ensemble 3. Identify the differences in the input/output files for DLMONTE 4. Illustrate the use of the Grand Canonical ensemble 5. Change input parameters to optimise results | | |
| Assumed knowledge? | | | From previous sessions:  Basic Monte Carlo theory and methodology, ensembles and use of DLMONTE program.  Thermodynamics – Chemical potential | | |
| Timings /min | ILO | | Teacher activity | Learner activity | Resources |
| 0-20 | 1, 2 | | Lecture on GC ensemble. | Listen. | Powerpoint slides:   * Definition * uses * comparison with other ensembles |
| 20-120 | 3, 4, 5 | | Provide guidance on exercises, either on an individual or group basis as appropriate. | Work through the practical exercises (based on tutorial 4 of workshop). | Self-contained tutorial on phase transitions on Lennard-Jones phase transitions using NVT ensemble, either as a Jupyter notebook or a pdf/html document. Will need input files and scripts. Simple answer sheet/guide for demonstrators. |