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| Session title: | | Introduction to the DLMONTE program | | | Course: MC2001 |
| Aims: | | Introduce the DLMONTE program  Use practical examples using DLMONTE to simulate phase transitions in a Lennard-Jones material  Introduce the concept of ensembles and move types, specifically in NVT and NpT. | | | |
| Intended learning outcomes (ILOs) : | | | 1. Describe some functions of the DLMONTE program 2. Define the primary DLMONTE i/o parameters 3. Recall how to run an MC simulation on DLMONTE 4. List the different move types available in NVT and NpT ensembles 5. Compare the use of NVT and NpT ensembles in solving problems 6. Illustrate and interpret output data from DLMONTE 7. Change DLMONTE input parameters to optimise results | | |
| Assumed knowledge? | | | Monte Carlo methodology and classical potential modelling from previous sessions  Appreciation of results from previous sessions  Thermodynamics-phase transitions | | |
| Timings / min | ILO | | Teacher activity | Learner activity | Resources |
| 0-10 | 1 | | Lecture on DLMONTE program. | Listen. | Powerpoint slides:   * overview * uses * capabilities |
| 10-45 | 2, 3, 6 | | Provide guidance on practical tutorial, either on an individual or group basis, as appropriate. | Work through practical exercise: follow the tasks, comprehend instructions, reflect on instructions, obtain and analyse results. Reflect on meaning of results. | 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. |
| 45-60 | 4, 5 | | Lecture introducing ensembles and move types. | Listen. | Powerpoint slides:   * ensemble averaging, * NVT and NpT ensembles, * translational and volume move types. |
| 60-120 | 3, 5, 6, 7 | | Provide guidance on practical tutorial, either on an individual or group basis, as appropriate. | Continue to work through practical exercise: follow the tasks, comprehend instructions, reflect on instructions, obtain and analyse results. Reflect on meaning of results. | Self-contained tutorial on phase transitions on Lennard-Jones phase transitions using NpT ensemble and volume moves, either as a Jupyter notebook or a pdf/html document. Will need input files and scripts. Simple answer sheet/guide for demonstrators. |