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| Session title: | Introduction to Molecular Dynamics simulations | | | | Course: MC2001 |
| Aims: | Introduce classical potential modelling methods  Introduce the concepts of molecular dynamics (MD)  Use practical examples to guide participants in running an MD simulation | | | | |
| Intended learning outcomes (ILOs) : | | | 1. Describe the approximations used in classical modelling 2. Define MD methodology 3. Identify the roles of kinetic and potential energy in MD models 4. Apply MD methods to model the solid-liquid phase transition of a Lennard-Jones material | | |
| Assumed knowledge? | | | Basic thermodynamics-phase transitions, energy in systems  Intermolecular forces-Van der Waals | | |
| Timings / min | | ILO | Teacher activity | Learner activity | Resources |
| 0-15 | | 1, 2 | Lecture on MD methodology. | Listen. | Powerpoint slides:   * quantum vs. classical model * MD methodology * history * motivation for use |
| 15-45 | | 2, 3, 4 | 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 as a Jupyter notebook or a pdf/html document. Will need DLPOLY input files and scripts. Simple answer sheet/guide for demonstrators. |
| 45-60 | | 3 | Lecture expanding on kinetic and potential energy in MD. | Listen. | Powerpoint slides:   * moving around an energy landscape in MD * reminder of kinetic theory and thermodynamics of phase transitions |
| 60-120 | | 2, 3, 4 | 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 as a Jupyter notebook or a pdf/html document. Will need appropriate input files and scripts. Simple answer sheet/guide for demonstrators. |