MDANSE 2018 – Sept. 24th - 28th 2018

Programme Recommendations

E. Farhi - Aug 27th 2018

The tentative programme was circulated some time ago, and we worked to balance the organizers contributions. The programme can still be shuffled, but in order to properly prepare the lessons and tutorials, it is probably better to stick to the proposed schedule, and set a few recommendations. These recommendations are not directive. We have assigned lessons and practicals according to organiser's main focus, and exchanged suggestions. If you estimate you are not suited for what is proposed, tell me and we shall find a way to re-assign.

The main focus of the school is to present computational tools, and explain how information can be transferred to other tools (e.g. McStas) in order to build or envisage a full simulation workflow from the material/sample down to the virtual experiment results to mimic experimental measurements. The audience is very diverse (structure, dynamics, McStas users, modelling world, nuclear data, ...), so that lessons and practicals should address novice users, who will benefit from the expert users around.

MDANSE 2018   Materials and Neutron Scattering Instrument Modelling.

	Monday 24th	Tuesday 25th	Wednesday 26th	Thursday 27th	Friday 28th
08:45-9:00	Welcome				
9:00-9:45	Molecular Dynamics Miguel	Practicals: Sylvain Spin waves	Introduction to McStas Peter	McStas – samples Erik	Simulation pipe-lines Emmanuel
9:45-10:30	DFT lattice dynamics and MD Sanghamitra		McStas Instrument classes John	Advanced samples Erik	Tools for automation Peter
10:30-10:45	coffee break	coffee break	coffee break	coffee break	coffee break
10:45-11:30	SpinWaves for dummies Sylvain	Practicals: Thomas ASE	Practicals: Erik McStas Diffract. Laue	Practicals: Erik McStas/Structure	Practicals: John
11:30-12:15	Gaussian approximation Emmanuel	Oriented towards dynamics	Practicals: Peter McStas/TAS	Liquid, Powder and SX	VE: Lattice dynamics – TAS/ToF
12:00-14:00	lunch	lunch	lunch	lunch	lunch
14:00-14:45	Practicals: Miguel MD: liquids and powders	Excursion to Teide	Practicals: John McStas/ToF	Practicals: Emmanuel	Practicals: Sanghamitra VE: Molecular Spec.
14:45-15:30			Practicals: Miguel McStas/QENS	McStas: Liquids, powders dynamics	– ToF/TOSCA/Lagrange
15:30-15:45	coffee break		coffee break	coffee break	coffee break
15:45-16:30	Practicals: Sanghamitra Lattice dynamics		Practicals: Sanghamitra McStas Instr:	Practicals: Peter McStas: SX dynamics	Practicals: Emmanuel VE: Gaussian approx – ToF
16:30-17:15	phonons in crystals		Molecular Spectroscopy		
	Sunday 23rd	Registration at the Hotel		Saturday 29th	Bye Bye
~ 20:00	lunch	lunch	lunch	lunch	lunch

The schedule includes lessons (in magenta) and practicals (in green), split into e.g. 45 minute slots. As there are many things to present, please make sure you will not exceed your allocated time, to leave the

coffee breaks safe. Practicals are of course more relaxed. We aim to have rather short days, to allow a friendly and enthusiastic exchange between all of us in time-off activities (beach, visits, drinks, …).

There are in total 36 slots, split into 10 lessons, and 15 practicals (usually 2 slots each). So the school is clearly hands-on oriented. Each lesson and practical will be based on a printed document (4 slides/page). **PDF's of these documents must be sent in advance by Sept 17th** at the latest to copy them on the USB keys, and pushed on the web sites. If possible, come with your printed copies (26 copies plus 2-4 for organisers/safety margin).

In terms of software, all students will be given a VirtualBox machine with pre-installed software on a USB key. As of today, we have the following list:
- Ubuntu 16.04 based
- Mantid
- McStas and associated tools (cif2hkl, …)
- ASE and PhonoPy
- ABINIT
- VASP
- LAMMPS
- GROMACS
- QuantumEspresso
- Matlab (trial version)
- iFit
- LAMP
- SpinWave
- MDANSE (ex. nMoldyn)

If you have other requests, tell me so that the virtual machine can be enriched. The version for each software will be set from what is easiest to install, *i.e.* may not be the latest release, except if you have specific needs.

Miguel

Present the classical MD theory (potential, canonical ensembles, thermostats, Verlet integrator, …) and usual software used for this. Highlight approximations/limitations of the methodology. Perhaps as well a quick overview of the different data formats, and how they can be used/edited/exported for other purposes. A few test cases / examples to show what can be obtained, and estimate the required resources (CPU time, memory, storage, …).

Liaise with: Sanghamitra for MD.

Prepare a simple model system (water, ethanol, ...), and configure the MD calculator. Perform an energy minimization, a temperature equilibration, and a production run. Analyse the Log files to detect that all is fine (energy, pressure, …). Treat the trajectory with MDANSE to extract vDOS, $g(r)$, $S(q)$, $S(q,\omega)$, $F(q,t)$, diffusion coefficient, … The calculation should be run on a laptop, or small cluster.
Possibly, if using LAMMPS, it could be useful to use the *ase.calculators.lammpsrun* calculator and generate a MD trajectory <https://wiki.fysik.dtu.dk/ase/ase/calculators/lammpsrun.html>. Some examples are available at <https://gitlab.com/ase/ase/blob/master/ase/test/lammpsrun/>.

Do the same on a solid system and perform a powder average using MDANSE.

Liaise with: Thomas for ASE, and Sanghamitra for MD.

Explain how a McStas QENS spectrometer is built. Assemble a simple QENS instrument and run it. Generate some realistic resolution profiles (Q, ω).

Liaise with: Peter and Erik to check that some QENS spectrometers are available in McStas and usable.

Sanghamitra

Introduce DFT theory (quickly) and concentrate on the lattice dynamics and ab-initio MD. Highlight approximations/limitations of the methodology. Present usual tools (calculators), as well a quick overview of the different data formats, and how they can be used/edited/exported for other purposes. A few test cases / examples to show what can be obtained, and estimate the required resources (CPU time, memory, storage, …). Links with ASE and PhonoPy would also be welcome.

Liaise with: Emmanuel (can use PhonoPy through iFit) and Thomas (ASE if needed).

Aim 1: perform a DFT lattice dynamics calculation for a simple system (e.g. Al bcc or something similar). Explain how to generate the material model, and the calculator configuration files. Run the calculation steps (displacements). Import results (forces) and generate vDOS and dispersion curves along principal directions.

Aim 2: same study, this time with *ab-initio* MD. Explain how the trajectory can be converted into vDOS, *S(q), S(q,ω),* etc.

<u>Note</u>: if you need CASTEP, you need to request yourself a UK licence to get the Linux executable and pseudo-potentials so that they can be added into the virtual machine.

Liaise with: Emmanuel (can use PhonoPy through iFit and ASE) and Thomas (ASE if needed).

Practical - Wednesday 26th 15:45-17:15 – McStas Molecular Spectroscopy (TOSCA, Lagrange, …)

Present the design concepts for molecular spectroscopy instruments, and identify the elements in a McStas model. Demonstrate how such instrument can measure some estimate of a density of states. Have students estimate the resolution and main spurions while running the McStas model.

Demonstrate how the ABINS Mantid Algorithm can model an experimental data set from a DFT calculation.

Liaise with: Peter to check for a TOSCA model/usage.

Practical – Friday 28th 14-15:30 – Virtual Experiments: Molecular Spectroscopy – ToF/TOSCA/Lagrange...

Have student get the results from the lattice dynamics or MD, and input into the McStas model to reproduce an experimental data set. TOSCA and Lagrange models can be used.

Liaise with: Peter to check for a TOSCA model/usage, Emmanuel to generate Sqw tables.

Sylvain

Lesson – Monday 24th 10:45-11:30 – Spin Waves: theory and usage

Present spin-wave calculation theory. Present the SpinWave software and its usage: input / output. Explain a methodology to export the result as an S(q,w) table.

Propose a simple spin-wave system. Explain how the input file is built, and identify the main parameters in it. Run the calculation and plot results. Export tables in a simple (q,ω) table (HKL line/plane/volume).

Liaise with: Emmanuel to format the SpinWave output into a format to be used by e.g. McStas.

Emmanuel

Lesson – Monday 24th 11:30-12:15 – Gaussian approximation, theory and application

Present the incoherent Gaussian approximation and explain how this can be used to estimate the $S_{inc}(q,w)$ for isotropic systems. Explain how the coherent scattering law can also be estimated. Show how it can be used to model most materials, e.g. from nuclear data bases.

Liaise with: Peter to help polish a little, Miguel.

Practical - Thursday 27th 14-15:30 – McStas sample dynamics: liquids and powders

Use *Isotropic_Sqw* sample McStas component to input a $S(q,\omega)$ table from e.g. MD. Look into the data format. Show how to extract scattering contributions. Identify limitations.

Liaise with: Peter, Sanghamitra and Miguel.

Lesson – Friday 28th 9-9:45 – Simulation pipe-lines

Identify the sources of information (structure, dynamics, experiments, modelling) and sketch for each how a path can be derived towards a full virtual experiment. Present the data formats, and possible tools/converters to build the pipe-line.

Liaise with: Miguel and Peter.

Practical – Friday 28th 15:45-17:15 – Virtual Experiments: Gaussian approximation - ToF

Start from a vDOS or gDOS and see how far we can go. Check for the validity of the approach. Experiment how we can import an ENDF material, and check its consistency.

Liaise with: Miguel.

Peter

Lesson – Wednesday 26th 9-9:45 – Introduction to McStas

Present McStas, and focus on how instruments are built. Present quickly the different types of components.

Liaise with: Erik

Practical - Wednesday 26th 11:30-12:15 – McStas TAS

Show how a TAS model can be assembled (based on the existing TAS tutorial). Estimate the resolution function, and compare with analytical models. You may use ResCal or ResLibCal for that.

Liaise with: Emmanuel and Erik.

Practical - Thursday 27th 15:45 – McStas sample dynamics: SX

Hard stuff: demonstrate how we can stack e.g. a SX structure model (SX component) with an other sample model to get 'some' SX dynamics (phonon_simple, incoherent scatterer, ...). Perhaps we can make Duc Le component work ? Would then only use the existing show case.

Liaise with: Emmanuel and Erik to experiment the Duc Le component.

Lesson – Friday 28th 9:45-10:30 – Tools for automation

Present the tools that can be used to build script/automate the pipe-lines, taking as operators the available software. This is mostly some Bash/Python/Matlab/McStas… scripting.

Liaise with: Emmanuel to sync with the pipe-lines.

Erik

Practical - Wednesday 26th 10:45-11:30 – McStas diffractometers: powder, SX, Laue

Have participants simulate a powder diffractometer, a SX diff, a Laue diff. Concentrate on the instrument model, not the sample. Estimate the Q-resolution from the peak shape *vs* scattering angle.

Liaise with: Emmanuel, Peter and Jon.

Lesson – Thursday 27th 9-9:45 – McStas sample components

Present most important sample components: physics/theory, limitations, use cases. For each, focus on main component parameters and display a typical syntax/application/result.

Liaise with: Peter (from Bariloche slides) and Emmanuel.

Lesson – Thursday 27th 9:45-10:30 – McStas advanced samples (combining, interfacing…)

Present the 'advanced' samples, that is those that produce the most realistic data to be inserted into a virtual experiment. Also present ways to combine different sample 'kernels' to add complexity. This may include the Union (but currently limited to structure, no dynamics). Also present ways to 'interface' sample with external codes (open question…), such as *cif2hkl*, etc.

Liaise with: Peter (from Bariloche slides) and Emmanuel.

Use the diffractometers presented on Wednesday in conjunction with an 'advanced' sample for diffraction, e.g. PowderN and Single_Crystal. Add incoherent background. Study how the scattering and peak shape evolve with the wavelength (scan). Do the sample with liquids, using the *Isotropic_Sqw* but detecting all energies.

Liaise with: Peter and Emmanuel.

Jon

Lesson – Wednesday 26th 9:45-10:30 – Instrument classes in McStas: a tour

Present the different classes of instruments available in McStas. Explain how to use, then customise such instrument models.

Liaise with: Peter (from Bariloche slides)

Practical – Wednesday 26th 14-14:45 – McStas time of flight spectrometers

Assemble a simple inelastic scattering instrument. Study its resolution in (q,w) using a Dirac peak sample.

Liaise with: Peter and Emmanuel.

Practical – Friday 28th 10:45-12:15 – Virtual Experiments: lattice dynamics TAS/ToF

Input results from lattice dynamics (or spin-waves) into a McStas spectrometer. This will most probably require to perform a 2D 'powder' average. Add incoherent scattering and structure S(q).

Liaise with: Emmanuel.

Thomas

Practical – Tuesday 25th 10:45-12:15 – Presentation of ASE: general use, and application to material structure and dynamics for neutrons

Use ASE to build a model (Atoms) either from a file (CIF, PDB, ...) or by adding single atoms and applying operators. Instantiate a Calculator, and demonstrate how to extract usual quantities (energy, …), minimize the system, perform a MD and a lattice dynamics calculation (Phonons). Export results.

Liaise with: Sanghamitra (for CASTEP), Emmanuel (link with PhonoPy via iFit), Miguel (classical MD, LAMMPS).