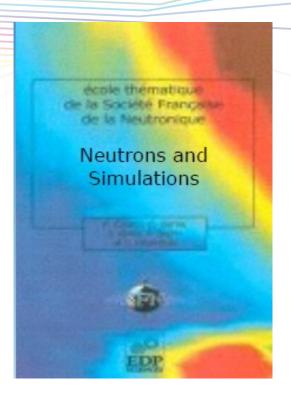




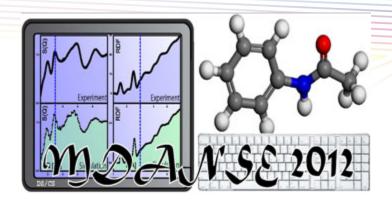
## 2010: School 0

- 18<sup>th</sup> Journées de la Diffusion Neutronique (organized by SFN – French Neutron Society)
- School 'Neutrons et simulations'





## **2012: MDANSE I**



- First school organized at ILL
- 3 days (March 2012)
- 30 participants
- Goal: First introduction to simulation techniques (overcome activation energy and loose fear)



## **2014: MDANSE II**

- Satellite event of QENS-WINS conference in Autrans
- 2 days (May 2014)
- Focus on QENS and inelastic neutron scattering

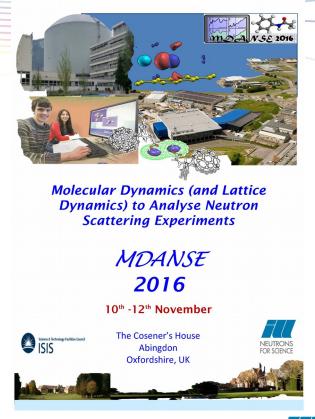




## **2016: MDANSE III**

- Co-organized by ILL and ISIS
- 2 days (November 2016)
- Included some advanced topics
- Proceedings: RAL-TR-2016-018







## **2018: MDANSE IV**











- Organizers/lecturers:
  - Emmanuel Farhi (ILL)
  - Sanghamitra Mukhopadhyay (ISIS)
  - Peter Willendrup (ESS/DTU)
  - Thomas H. Rod (ESS)
  - Erik Knudsen (DTU)
  - Miguel A. Gonzalez (ILL)
  - Felix Fernandez-Alonso (ISIS)
  - Jon Taylor (ESS)
- 1 week
- Intro to simulation Virtual experiments



## **2018: MDANSE IV**

(My view)

#### Still a school:

- Some (few) lectures
- Plenty of time for hands-on practicals and discussions
- Do not hesitate to ask questions and request help

### But also kind of a workshop:

- We are all exploring ways of facilitating the integration of simulation tools with experiment
- Discuss, tell us what tools you use, which things work or not, ...
- Propose alternative ways of doing, applying, and analyzing simulations



## Learn, share, enjoy!



# Organizers

- E. Farhi (ILL)
- M. A. Gonzalez (ILL)
- S. Mukhopadhyay (ISIS)
- T. Rod (ESS/DMSC)
- P. Willendrup (ESS/DTU)
- E. Knudsen (DTU)
- J. Taylor (ESS/DMSC) [excused]
- F. Fernandez-Alonso (ISIS) [excused]
- •
- Contact: mdanse2018@ill.fr
- http://mdanse2018.essworkshop.org/

# Made possible with

- Your generous registration!
- **SINE2020** (Grant 654000-SINE2020- H2020-INFRADEV-2014-2015/H2020-INFRADEV-1-2014-1)
- ISIS
- ILL
- DTU
- ESS









MDANSE 2018		Materials and Neutron Scattering Instrument Modelling.			
İ	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	Practicals: Peter McStas/ToF	McStas – samples <mark>Erik</mark>	Simulation pipe-lines Emmanuel
9:45-10:30	MD Sanghamitra		Practicals: Miguel McStas/QENS	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: Sanghamitra McStas Instr:	Practicals: Erik McStas/Structure	Practicals: Emmanuel
11:30-12:15	Gaussian approximation Emmanuel	Oriented towards dynamics	Molecular Spectroscopy		VE: Lattice dynamics – TAS/ToF
12:00-14:00	lunch	lunch	lunch	lunch	lunch
<b>/</b>	Practicals: Miguel	Introduction to McStas	,	Practicals: Emmanuel	Practicals: Sanghamitra
14:00-14:45	MD: liquids and powders	Peter	Excursion to Teide		VE: Molecular Spec.
14:00-14:45 14:45-15:30			Excursion to Teide	McStas: Liquids, powders dynamics	
	MD: liquids and powders	Peter McStas Instr. classes	Excursion to Teide	McStas: Liquids,	VE: Molecular Spec.
14:45-15:30	MD: liquids and powders  coffee break  Practicals: Sanghamitra	Peter McStas Instr. classes Erik coffee break Practicals: Erik McStas Diffract. Laue	Excursion to Teide	McStas: Liquids, powders dynamics	VE: Molecular Spec ToF/TOSCA/Lagrange
14:45-15:30 15:30-15:45	MD: liquids and powders  coffee break  Practicals: Sanghamitra	Peter McStas Instr. classes Erik coffee break Practicals: Erik	Excursion to Teide	McStas: Liquids, powders dynamics coffee break Practicals: Peter	VE: Molecular Spec.  - ToF/TOSCA/Lagrange coffee break Practicals: Emmanuel
14:45-15:30 15:30-15:45 15:45-16:30 16:30-17:15	coffee break Practicals: Sanghamitra Lattice dynamics phonons in crystals	Peter McStas Instr. classes Erik coffee break Practicals: Erik McStas Diffract. Laue Practicals: Peter		McStas: Liquids, powders dynamics coffee break Practicals: Peter	VE: Molecular Spec.  - ToF/TOSCA/Lagrange coffee break Practicals: Emmanuel
14:45-15:30 15:30-15:45 15:45-16:30 16:30-17:15	coffee break Practicals: Sanghamitra Lattice dynamics phonons in crystals	Peter McStas Instr. classes Erik  coffee break Practicals: Erik McStas Diffract. Laue Practicals: Peter McStas/TAS		McStas: Liquids, powders dynamics coffee break Practicals: Peter McStas: SX dynamics	VE: Molecular Spec.  - ToF/TOSCA/Lagrange coffee break Practicals: Emmanuel VE: Gaussian approx - ToF