

FARHI Emmanuel

Born August 21st 1970, French
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married, 4 children ; farhi(at)ill.fr

Master in Physics Engineering, Ph.D. in Physics
M.Sc. in Laser Physics
Scientist in neutron scattering, specialized in scientific computing

Education

- 1995-1998 : PhD in Montpellier II University, with Highest Honors
- 1993-1994 : MSc2 in Laser-Matter interaction, Paris XI University, France
- 1990-1994 : Master Engineer Diploma from the Ecole Supérieure de Physique et de Chimie Industrielles de la ville de Paris (E.S.P.C.I.), 10 rue Vauquelin, 75005 Paris, France. (Physics and Chemistry)

Skills

- Languages: French (mother tongue), English (fluent), Spanish (medium), Japanese (bases), Swedish (bases).
- Computing systems: Linux, Unix, Windows, MacOS
- Computing languages: C, Fortran, Perl, HTML, XML, LeX/Yacc, Matlab/Scilab, IDL, Labview, Python
- Instrumentation: GPIB, Mechanics, Lasers, neutron optics
- Science: solid and liquid state physics, biology, neutron scattering, Brillouin light scattering molecular dynamics, optimisation, signal processing

Scientific and working experience

2001-2013: 'Computer scientist' at the ILL

- Structure and dynamics of liquid and solid ^4He (J. Bossy, E. Polturak, H. Glyde)
- Simple liquids study: experiments, *ab-initio* simulations (indium, rubidium, gold, cadmium, caesium, ...), collaboration with U. Bafile, E. Guarini
- Development of McStas <http://www.mcstas.org> with K. Lefmann, P. Willendrup.
- Simulation of neutron spectrometers by Monte Carlo technique. I have simulated about 42 ILL instruments and experiments in the last 7 years.
- Development of data analysis tools (Matlab, IDL, C), <http://ifit.mccode.org>
- Simulation of cold moderators (liq-D2 and H2, water, 4He, ...) including complex geometries (inserts/groove, slabs, ...)
- Ionizing radiation tolerant algae study with C. Rivasseau (CEA Grenoble). 3 Patents.
- Handling and development of the Spin Echo option for the IN20 Thermal Triple Axis neutron instrument (C. Zeyen, J. Kulda, M. Enderle)

1998-2001: Second instrument responsible for the IN20 spectrometer at the ILL

- Handling and development of the IN20 Thermal Triple Axis neutron instrument (J. Kulda, J. Locatelli)
- Handling of the Cryopad (neutron polarimetry) option for the IN20 Thermal Triple Axis neutron instrument (F. Tasset)
- Handling and development of the Spin Echo option for the IN20 Thermal Triple Axis neutron instrument (C. Zeyen, R. Aabel)
- Superfluid 4He roton dynamics using spin-echo measurements (B. Fak)
- Simulation of neutron spectrometers by Monte Carlo technique (K. Nielsen, K. Lefmann, I. Anderson)
- Development of data analysis tools (MFit)

1995-1998: PhD with E. Courtens, A.K. Tagantsev, R. Currat

- Quantum paraelectric anomaly study in KTaO₃ perovskite (Laboratoire des Verres, Montpellier II University, France)
- MSc1 teaching at Montpellier II University (optics, mechanics)

1994-1995: Military Duty as Scientist in Special Materials

- Thin film study by electrochemical and optical analysis P. Topart (CEA/DAM, Centre d'Etude du Ripault, Tours)

1992-1994: Education Training

- MSc2 Laser-Matter interaction: Laser produced silver metallic clusters, trapped in low temperature rare gas matrix, studied by dichroic optical spectroscopy J.C. Rivoal (Laboratoire d'Optique Physique, E.S.P.C.I., France)
- Neural Network regulation of complex processes R. Dreyfus (Laboratoire d'Electronique, E.S.P.C.I. France)
- Acid-base properties of oxide-glass interfaces H. Arribart, X.Y. Lin (Laboratoire Mixte C.N.R.S, Saint Gobain Recherche, Aubervilliers, France)
- Semiconductor fluorescence (Monastir, University, Tunisia).

Main activities

Structure and dynamics of liquid and solid ^4He

I have get involved in the study of liquid helium when the IN20 spin-echo option was used to measure the life-time of the elementary excitation, in year 2000. Liquid helium is a model quantum liquid, which exhibits numerous original features: a single, very sharp single excitation dispersion branch, no pure elastic scattering, a strong 'roton' excitation which behaves as a Bragg peak in a liquid, a continuum of multi-phonon excitations above the elementary excitation, and many others. I have taken part in neutron inelastic scattering experiments to measure its dispersion and life-time with very high accuracy. As a model material, I have been using liquid helium to benchmark neutron scattering kernels used in McStas. This cryogenic liquid can also be used as a neutron cold moderator, to produce ultra-cold neutrons.

Solid helium, in cubic and hexagonal phases, is a quantum solid model material. It also exhibits many unique features. I have taken an active part in many experiments using high resolution triple axis spectrometers (IN14, IN12, S42), to explore the dispersion curves in the solid helium cubic phase.

Simple liquids study: experiments, *ab-initio* simulations (indium, rubidium, gold, cadmium, caesium, ...)

I have undertaken a systematic study of mono-atomic liquid metals, as part of a benchmarking procedure for the isotropic inelastic scattering kernel in McStas. I used *ab-initio* molecular dynamics codes, such as VASP and CASTEP, then process the trajectories with nMoldy, to extract the dynamic structure factors. The dynamic structure factor of Ag, Al, Au, Bi, Cd, Cs, Cu, D₂O, D₂, Ga, H₂O, ^4He , In, Li, Nb, Pb, propanol, Rb, Se, Si, Sn, Ti, Tl, V, Zn have been obtained. Very few publications include raw measurements that can be used to test single coherent and incoherent, multiple scattering and sample environment contributions. Rubidium and caesium are two of these. I then searched for materials which could be measured using thermal-cold neutrons, to provide new results. The dynamics of indium has never been measured with neutrons, due to its high absorption, and very low scattering power. An experiment was requested, based on a virtual experiment modelling which demonstrated that features could be measured. It was supplemented with a virtual experiment for the interpretation of the measurements. Similarly, the dynamics of liquid silver, cadmium and gold has been investigated, both experimentally and by means of virtual experiments.

Development of McStas <http://www.mcstas.org>

I have been using the McStas software since 1999. I gradually contributed to the code, and am now officially part of the development team, The main achievements in this field have been the development of advanced scattering kernels, especially the inelastic isotropic material one, the ability to transparently use large high performance computing clusters, the any-shape geometry for most samples and some advanced neutron optics components, as well as improvements to the grammar which is used to describe instruments and components, and the support for NeXus files. Since the early days of McStas, a community of users has appeared, which now contribute actively to the software.

Simulation of neutron spectrometers by Monte Carlo technique.

I have simulated about 42 ILL instruments and experiments in the last 7 years, as well as other instruments elsewhere.(LLB, HZB, ESS, ChalkRiver,). Most of these have been made available to

the community in the McStas distribution. Instrument models are often extended with samples to simulate virtual experiments.

Development of data analysis tools and iFit <http://ifit.mccode.org>

I have participated to various data analysis tools developments since my Ph. D. These were originally written in Matlab and C. When joining the Computing for Science group at the ILL in year 2000, I took over the Light instrument control interface (sister from Lamp). One of its innovations was to perform a data analysis while the experiment was running, in order to optimize the counting time by defining a statistical criteria to end the current acquisition and proceed to the next.

As a complement to McStas, the need for a flexible, generic data analysis infrastructure providing advanced mathematical operators made me start the iFit project. It is the result of 2 previous prototypes. It can be used to import/export many different data formats, including McStas and any NeXus flavour. A key feature resides in its optimisation routines, which can for instance be used to include a virtual experiment in a fitting loop.

Simulation of cold moderators (liq-D2 and H2, water, 4He, ...) including complex geometries (inserts/groove, slabs, ...)

I have taken part into a collaborative effort to optimize neutron moderators. These devices can be simulated with MCNP and McStas, even with complex geometries. However, the low energy thermalisation process can not be accurately modelled with MCNP, as this code lack dynamical and structural information for most cold moderator. Benefiting from the McStas project, I have gradually enriched the dynamical and structural information for water and cryogenic materials such as liquid deuterium, hydrogen and helium. It is then possible to study and optimise the neutron cooling process. This data is currently be made available for MCNP.

Ionizing radiation tolerant algae study

I have discovered, by chance, an ionizing radiation tolerant algae, which also has the ability concentrate metals and radio-isotopes. In collaboration with CEA, this algae has been identified from its RNAr sequence, and named *Coccymyxa actinabiotis*. Numerous studies are under way to understand the metal accumulation capabilities and the radio-resistance mechanisms. Potential applications of this algae for water cleaning, including in case of nuclear accident, are protected by 3 patents. A pilot plant has been set-up to evaluate the efficiency of this bio-technology. This study has used neutron back-scattering, diffraction (x-ray, neutron), EXAFS/XANES, X-ray fluorescence, PCR sequencing, NMR, ICP-MS, chromatography.

Instrumentation

I have assembled a Brillouin light scattering spectrometer during my Ph. D. After joining the ILL, I was responsible for the IN20 triple-axis spectrometer at the ILL, and participated in the instrumentation of its spin-echo option.

Publication list

1. “Advanced sources and optical components for the McStas neutron scattering instrument simulation package”, E Farhi, C Monzat, R Arnerin, T Van Vuure, C Castán-Guerrero, C Hennane, P A Harraud, G Campioni, S Fuard, J Ollivier, P Willendrup *Journal of Neutron Research* 17 (2013) 63.
2. “Dynamics of liquid Au from neutron Brillouin scattering and ab initio simulations: Analogies in the behavior of metallic and insulating liquids”, E. Guarini, U. Bafile, F. Barocchi, A. De Francesco, E. Farhi, F. Formisano, A. Laloni, A. Orecchini, A. Polidori, M. Puglini, and F. Sacchetti , *Phys. Rev. B* **88** (2013) 104201.
3. “Solid para-hydrogen as the paradigmatic quantum crystal: Three observables probed by ultrahigh-resolution neutron spectroscopy”, F. Fernandez-Alonso, C. Cabrillo, R. Fernández-Perea, F J. Bermejo, M. A. González, C. Mondelli, and E. Farhi, *Phys. Rev. B* **86**, (2012) 144524.
4. “Virtual experiments: Combining realistic neutron scattering instrument and sample simulations”, E. Farhi, V. Hugouvieux, M.R. Johnson, W. Kob, *Journal of Computational Physics* **228** (2009) 5251–5261
5. “Light and heavy water dynamic structure factor for neutron transport codes”, E. Farhi, G. Ferran, W. Haecck, E. Pellegrini, Y. Calzavara, *J. Nucl. Sci. Tech.* In Press, (2014)
<http://dx.doi.org/10.1080/00223131.2014.984002>