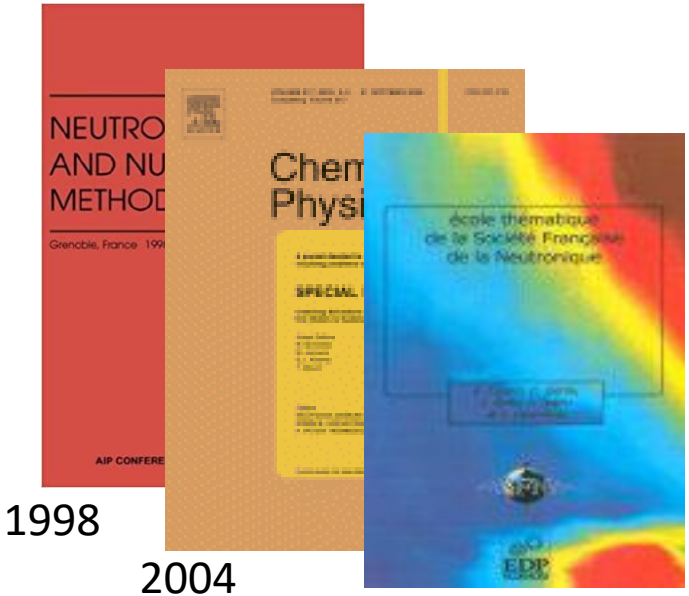
ESS/ILL User Meeting. Topical session on:

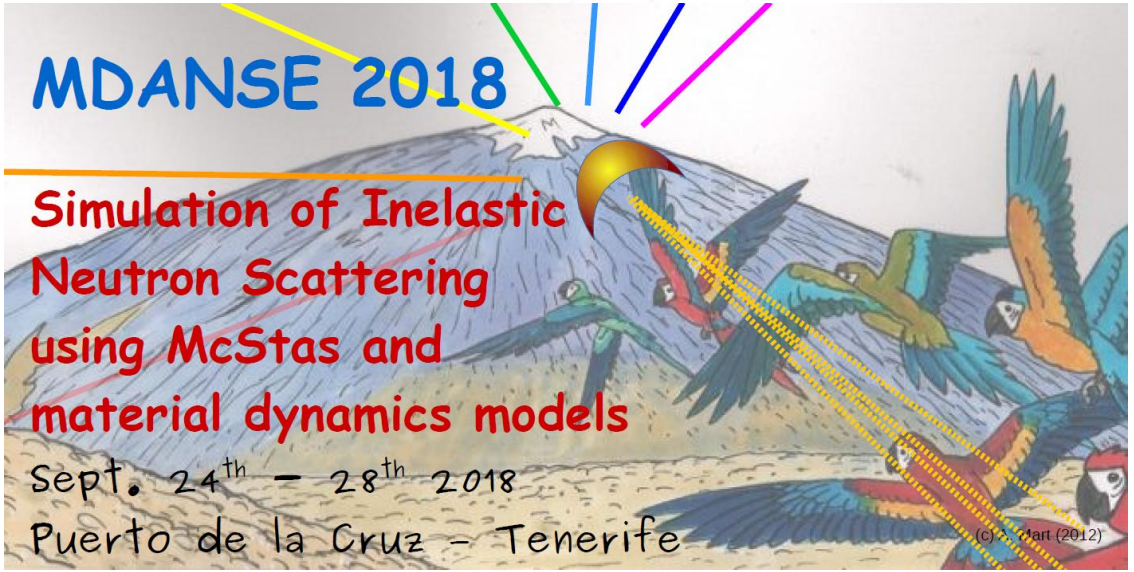
Atomic-scale simulations in neutron scattering

A quick look to the past (from an ILL perspective)

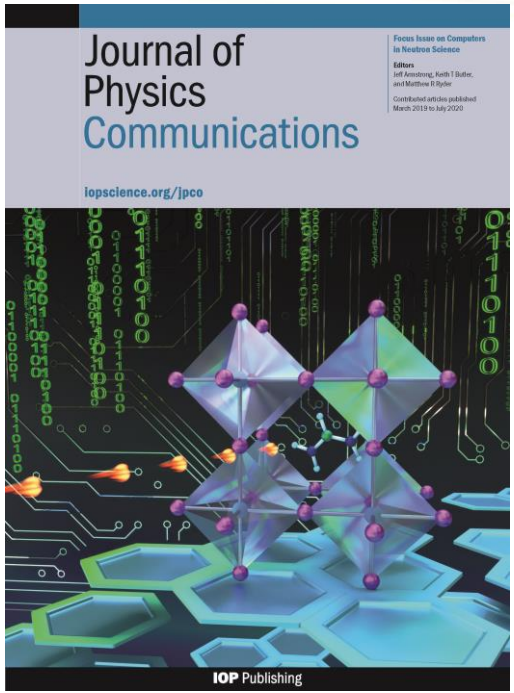
Around 1995, a small pioneering group formed around Don Kearley and Mark Johnson.
Goal: Foster and facilitate use of numerical simulations to complement neutron experiments.



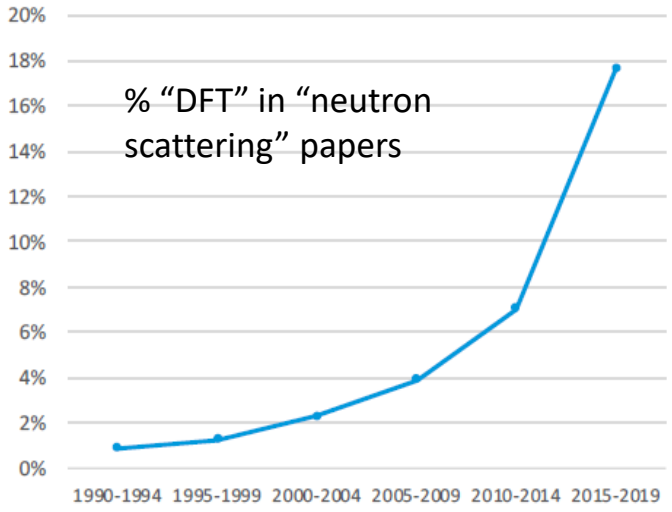
1998 2004 2010



The present



Focus Issue on Computers in Neutron Science (ISIS/ORNL editors, 2020)



The present: General tools

We (“neutron users”) benefit from:

- Hardware advances (more affordable computing power).
- Methods and software developed by specialized groups and made accessible to non specialists.

And during this workshop we heard of:

- New approaches to extend DFT to large systems of biological interest (Luigi Genovese and Viviana Cristiglio, Octav Caldararu).
- And multiple examples of techniques (DFT, classical MD, coarse-grained, ensemble optimization, …) and available software (Gromacs, Lammps, NAMD, Vasp, Castep, …) providing us with efficient tools to study very different types of scientific problems.

The present: Specific tools

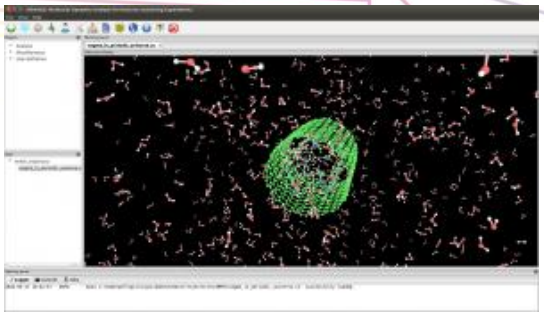
Less likely to find outside the software needed to calculate neutron observables.

*n*MOLDYN: A program package for a neutron scattering oriented analysis of Molecular Dynamics simulations

Gerald R. Kneller [a,b,1], Volker Keiner [c,2], Meinhard Kneller [c,3], Matthias Schiller [c,4]

[a] *IBM France, 68-76 Quai de la Rapée, F-75012 Paris, France*
[b] *DBCM SBPM, CEA, CE Saclay, F-91191 Gif-sur-Yvette, France*
[c] *Rheinische Friedrich-Wilhelms-Universität Bonn, Bonn, Germany*

Comp. Phys. Comm. (1995)



MDANSE: U. Orleans → ILL → ISIS

And here we learned about:

- MD2reflect (Nebojsa Zec)
- LiquidLib (Yanqin Zhai)
- “Private” analysis scripts/programs: Could they be useful to other neutron researchers?

The present: Applications

We have seen examples of applications in many different domains:

- Biology, with references to health issues (coronavirus, Alzheimer, Parkinson, Huntington, …)
- Materials: Energy materials (e.g. ILs and DES for battery electrolytes, ion conductors, thermoelectrics, …), nanotubes and nanopores, etc.
- Polymers and soft-matter
- Magnetism
- Fundamental science

And combined with most of the available neutron techniques:

- Neutron diffraction, small angle scattering, reflectivity
- Quasielastic and inelastic scattering

BROAD SCOPE (both of neutrons and simulations)

The present: Initiatives

Close collaboration between the scientific groups of the European neutron facilities:

- SINE 2020 – WP 10 (reduction and data analysis software, including simulations as a kind of advanced data treatment)
- PaNOSC – ViNYL (virtual experiments, including input from simulations)
- MDANSE school
- LENS (League of advanced European Neutron Sources):
  - WG4: Computing, Data → subgroup on computer simulations
    (Sanghamitra Mukhopadhyay, ISIS)

ANY FEEDBACK, SUGGESTION, CONTRIBUTION IS HIGHLY APPRECIATED

The future looks brilliant

- We had mainly young speakers (~50% PhD students) and the quality of the work and the presentations was really high.

KEEP DOING SUCH GOOD WORK AND I HOPE THAT MANY AMONG YOU WILL PURSUE A SCIENTIFIC CAREER AND FORM THE NEXT GENERATION OF NEUTRON SCATTERERS!

The future looks brilliant

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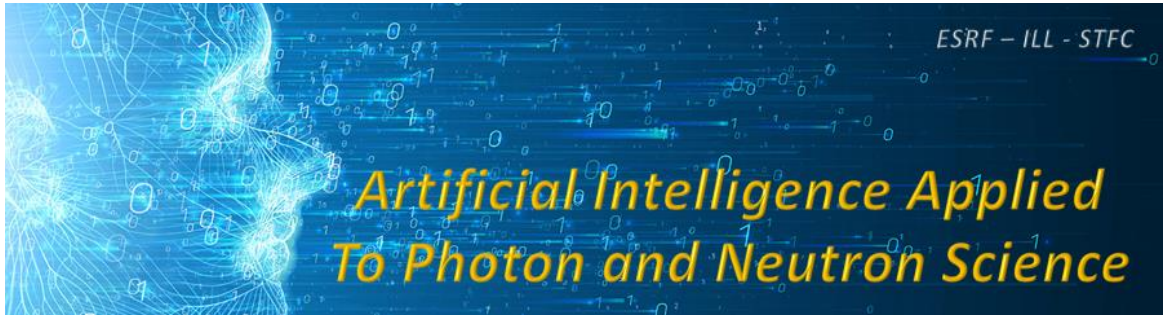
- New developments and methods continue to be developed, e.g. AI, ML, quantum comp, …



Workshop on Perspectives and Applications of Deep Learning for Accelerated Scientific Discovery at next generation X-ray and Neutron Sources

26-27 September 2019
August Krogh Building
Europe/Copenhagen timezone

The future looks brilliant

- We had mainly young speakers (~50% PhD students) and the quality of the work and the presentations was really high.
- New developments and methods continue to be developed, e.g. AI, ML, quantum comp, …
- ESS will soon be a reality

October 2020

First users in 2023!

The future looks brilliant

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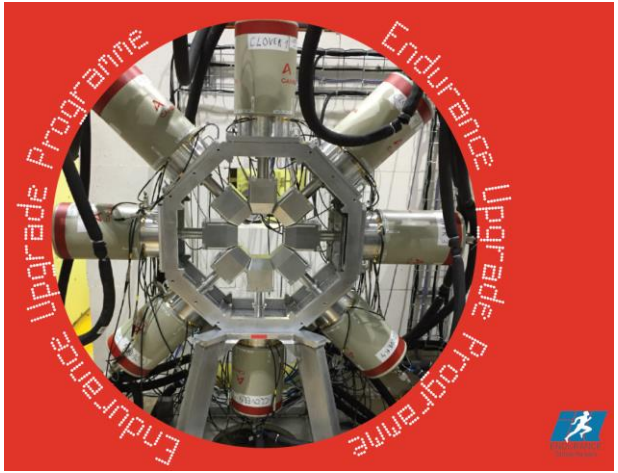
- New developments and methods continue to be developed, e.g. AI, ML, quantum comp, …
- ESS will soon be a reality
- And ILL remains in good shape



ENDURANCE PHASE 2: 2019

Endurance-2 projects were initiated with an open call at the start of 2017 and approximately 40 were received for a total budget of 60 M€. Following careful evaluation by the Instrument Sub-committee, the Scientific Council and the Steering Committee, two-thirds of the projects were retained for a budget of approximately 40 M€. This set of projects has been split into three parts, the first to be started in 2019 as detailed below.

PROJET	DESCRIPTION	DELIVERY
D11	Large area detector	2021
D22++	Wide angle detector	2021
D16	Wide angle detector	2021
D20c	Replacement detector	2021
IN20	Monochromator and multianalyser/detector	2021
LADI-B	Second protein crystallography station	2019
IM2020 -NeXT	Public imaging beam line	2020
H15	Guide design	2019
NESSE2	Sample environment equipment	2019 - 2023
BASTILLE2	Data treatment software	2019 - 2023

2030 and beyond!

The future looks brilliant

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- New developments and methods continue to be developed, e.g. AI, ML, quantum comp, …
- ESS will soon be a reality and ILL remains in good shape

Looking forward to meet you again in 2022!

And this time in Lund, and not on screen!