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PHOTONS AND NEUTRONS REALISTIC ARTIFICIAL INTELLIGENCE DATASETS (PaNRAID)

OBJECTIVE:

This course aims to develop an integrated approach to generating synthetic data for supervised learning, based on the combination of multi-scale material simulations (DFT, MD, XAS spectroscopy) and comprehensive digital twins of experimental X-ray and neutron facilities, including instrumental effects and experimental artefacts.

AUDIENCE:

This training course is intended for:

- Doctoral
- Post-doctoral students
- Teachers-research
- Researchers / research engineers

PREREQUISITES:

- English proficiency at B2 level (the training is delivered in English
- Basic knowledge of X-ray and/or neutron instrumentation is desirable, as well as of scientific data processing tools: numerical computation (Python, etc.) / simulation
- Personal laptop for practical sessions with software pre-installed McStas [https://mcstas.org/] and McXtrace [https://mcxtrace.org/].

PROGRAM:

Monday september 21st afternoon: Introduction

Presentation of the challenges involved in simulation for generating realistic data in supervised AI, as well as the key tools (McStas/McXtrace) used to model complete experimental setups.

Tuesday september 22st morning: Neutron and X-ray sources, detectors

Modelling of neutron and X-ray sources, as well as detector simulation.
Understanding how these elements influence the quality of experimental data and how to integrate them into virtual setups to generate realistic data.

Tuesday september 22st afternoon: Optics

Simulation of optical components used in experimental setups (lenses, mirrors, monochromators, etc.). The focus is on their role in signal formation and on how to model them to faithfully reproduce experimental artefacts.

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PROGRAM: (continued)

Wednesday september 23st morning: Diffraction samples

Study of numerical models of material samples that diffract neutrons and X-rays. Simulation of diffraction experiments by incorporating the physical properties of the materials to generate realistic datasets.

Wednesday september 23st afternoon: Spectroscopy samples

Modelling of samples for spectroscopy experiments (e.g. XAS). Simulation of interactions between radiation (neutrons/X-rays) and materials, in order to produce annotated and realistic spectroscopic data for training AI models.

Thursday septembre 24st morning: Imaging samples

Simulation of samples for imaging applications (CT scans, X-rays, etc.). Generation of virtual images incorporating experimental artefacts, in order to create varied and realistic datasets for supervised learning.

Thursday septembre 24st afternoon: AI applications: training

Presentation of methods for training supervised AI models using the simulated data generated previously. The focus is on using these realistic datasets to improve the robustness and generalisation of the models, taking into account the specific characteristics of the experimental setups.

Friday septembre 25st: AI Applications: Inference

Using the trained AI models to perform inference tasks on real or simulated experimental data.

The ultimate aim is to evaluate the performance of the models and discuss best practices for optimising their deployment in real-world application contexts.

TRAINEURS:

Peter WILLENDRUP :
Senior Research Engineer in the Department of Physics at the Technical University of Denmark (DTU), he is seconded to the Data Management and Scientific Computing Centre (DMSC) at the European Spallation Source (ESS).
Peter has led the development of McStas since 2002 and has been co-developing McXtrace since 2009.

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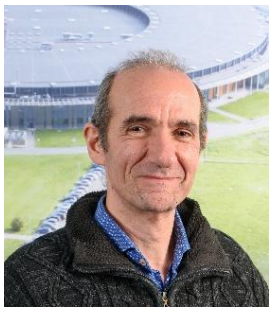
FRANCE 2030 PROGRAMME DE RECHERCHE MATÉRIAUX ÉMERGENTS

DIADEM Academy

TRAINEURS: (continued)



Emmanuel FARHI :
HEAD of the 'Data Reduction and Analysis' group at the SOLEIL synchrotron.
An expert in physics and materials science, Emmanuel is a key contributor to the McStas and McXtrace projects.

José Robledo :
Researcher at CONICET and lecturer at the Balseiro Institute in Argentina.
José, an expert in AI and neutron science, applies machine learning to the analysis of neutron data and develops simulated

SESSION :
21–25 September 2026:
CNRS CAES Village (St-Pierre d'Oléron)

DURATION :
5 days
8 half-days of training: 28 hours

MODALITY :
Présentiel

PRICE: €700
Included in the price:
Return shuttle bus to La Rochelle
Accommodation = 4 nights
Meals from the evening of the 21st to midday on the 25th
Bike hire package

Group outing (optional = €20 extra)

Information and registration:

Elodie ISTE :
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