ELI-ALPS Research Institute

TOWARDS THE SHARP END OF ATTOSCIENCE

Neutron diffraction from Boro-carbon for efficient structural analysis and defect detection

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SZÉCHENYI 2020

Hungarian Government

European Union
European Regional Development Fund

INVESTING IN YOUR FUTURE

Based on use case from WP5, PaNOSC

ELI-ALPS user facility

….with special thanks to all my WP5 colleagues

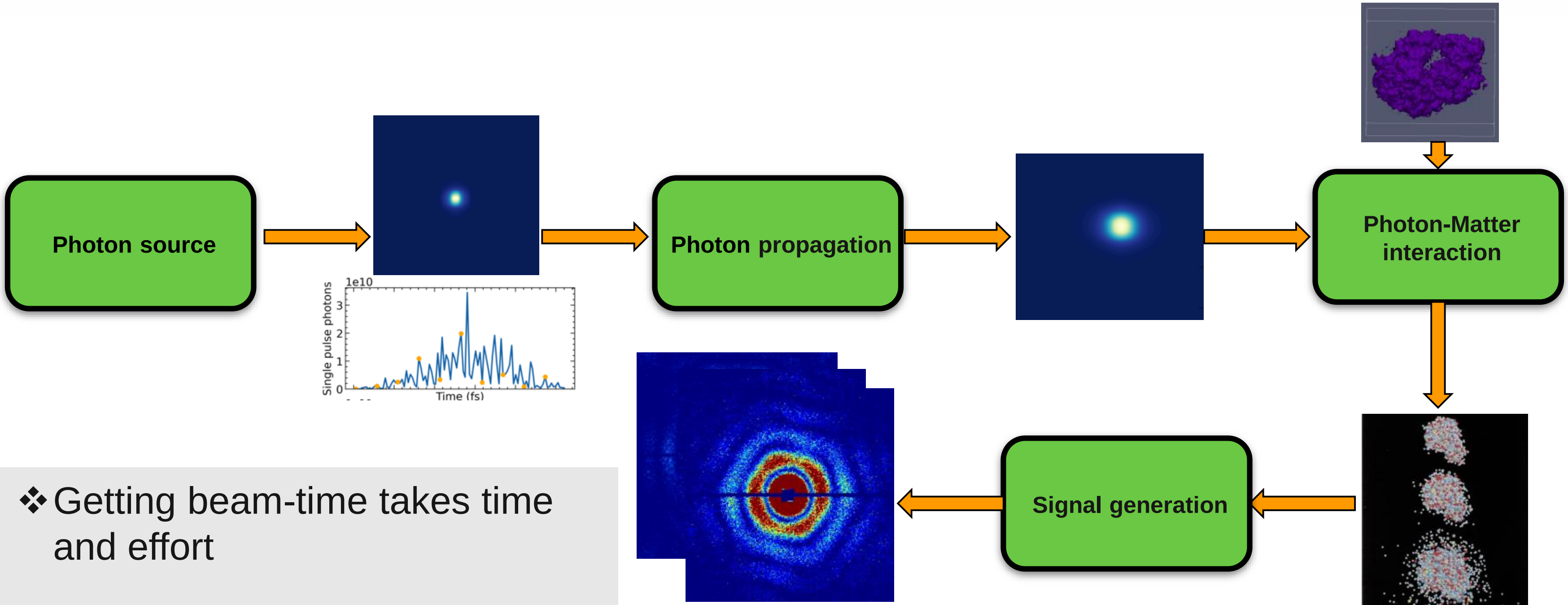
- Call: Horizon 2020 InfraEOSC-04
- Partners: ESRF, ILL, XFEL.EU, ESS, CERIC-ERIC, ELI-DC, EGI
- An European project for making FAIR data a reality, for **EOSC**

ESFRI European Strategy Forum on ResearchInfrastructures

ELI-ALPS **Szeged**
Hungary
Ultrashort laser pulses at high repetition rate

https://www.panosc.eu/all-use-cases/
Use case:18

What makes a successful user experiment?



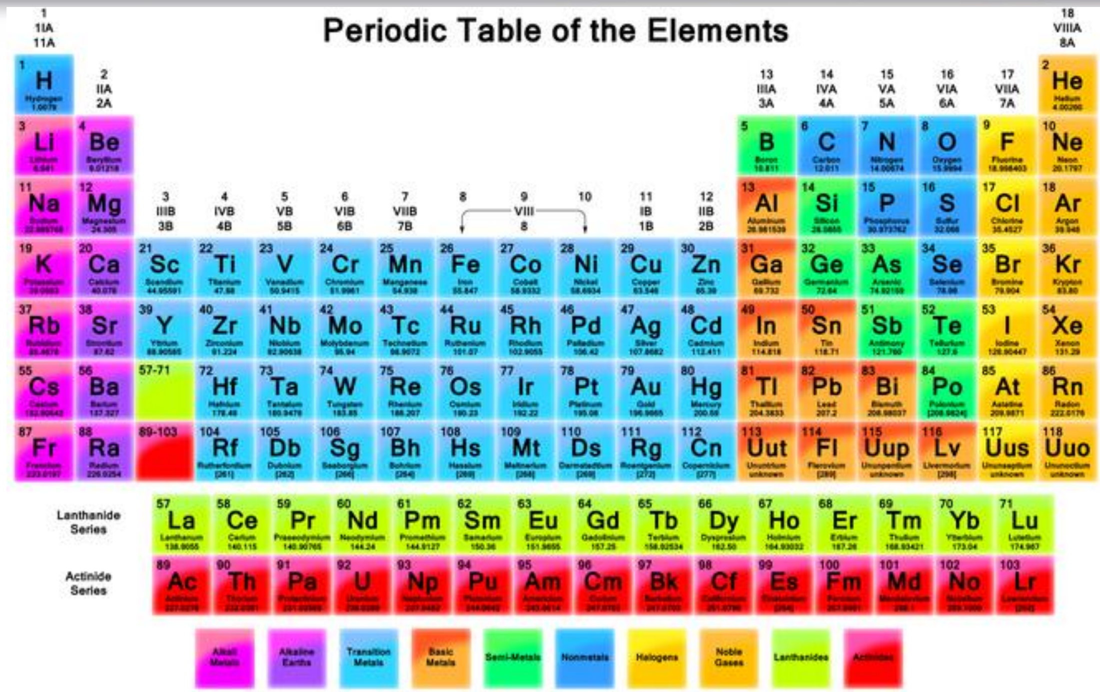
- Getting beam-time takes time and effort
- Finding optimal configuration of processes and resources reduces the time required for carrying out the experiment.
- Ensuring minimal idle time and maximal production is necessary.

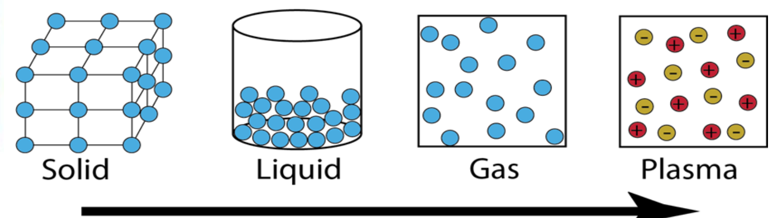
- What will happen during the interaction?
- Does that influence what can be measured on the detector?

Neutze, R., Wouts, R., van der Spoel, D., Weckert, E. & Hajdu, Nature 406, 752–757 (2000).
Yoon, C. H. et al. Scientific Reports 6, 24791 (2016).
Fortmann-Grote, C. et al. IUCrJ 4, 560–568 (2017).

Comuptation/simulation is **used for process analysis and process optimization.**

Use LASER to understand and control materials





Control and trace the motion of atoms in molecules

⇒ Control chemical reactions

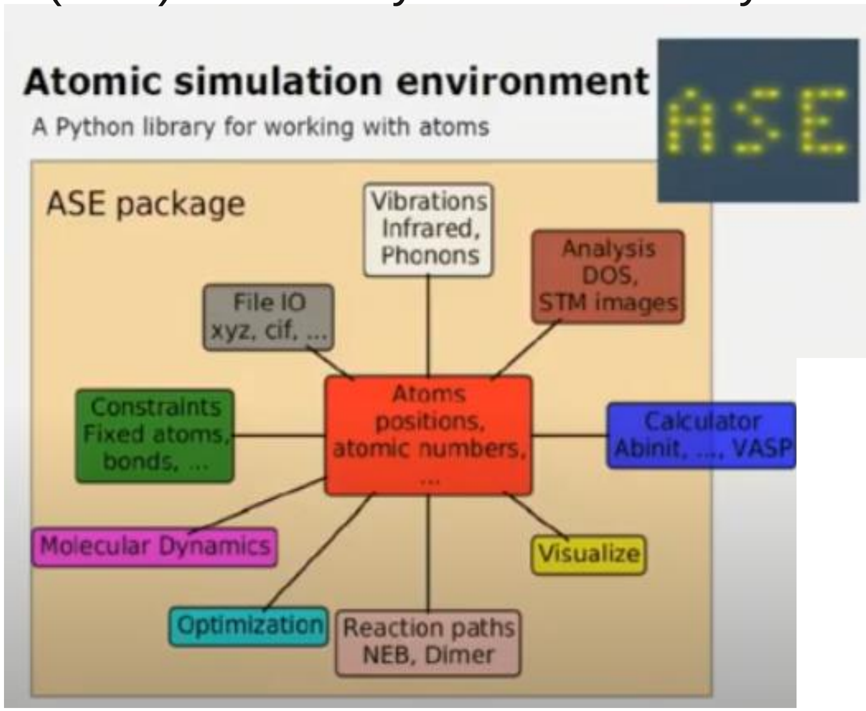
Control & trace electrons inside atoms & molecules

Femto

Atto

Within WP5 – combine ASE and McStas

Atomistic simulation environment (ASE) for Density functional study



Aim: Unified interface

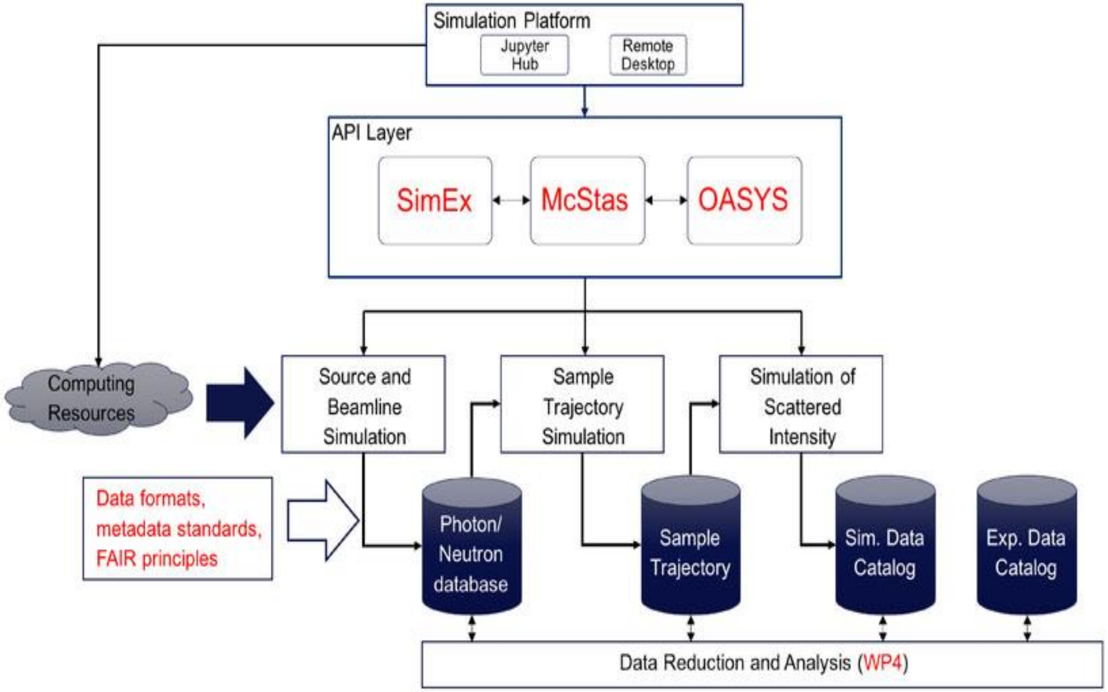
SimEx: flexible modular code to mimic an entire laser beamline.

McStas: Neutron beamlines

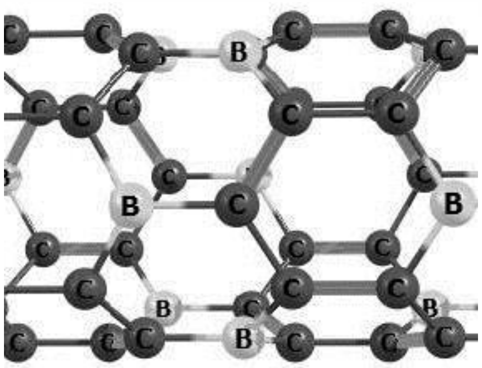
IMP: Interaction with materials

http://www.mcstas.org/about/

for modelling complex optics, using simple building bricks – example: represent a beamline



How this use case correlates to other projects….



Boro-carbon

conductive diamond electrodes for electrochemical detection

- Currrent use case- ASE + McStas - using a common platform
- FAIR Data Management -→ relates to ExPaNDs, IMPULSE

Use Case Action Flow

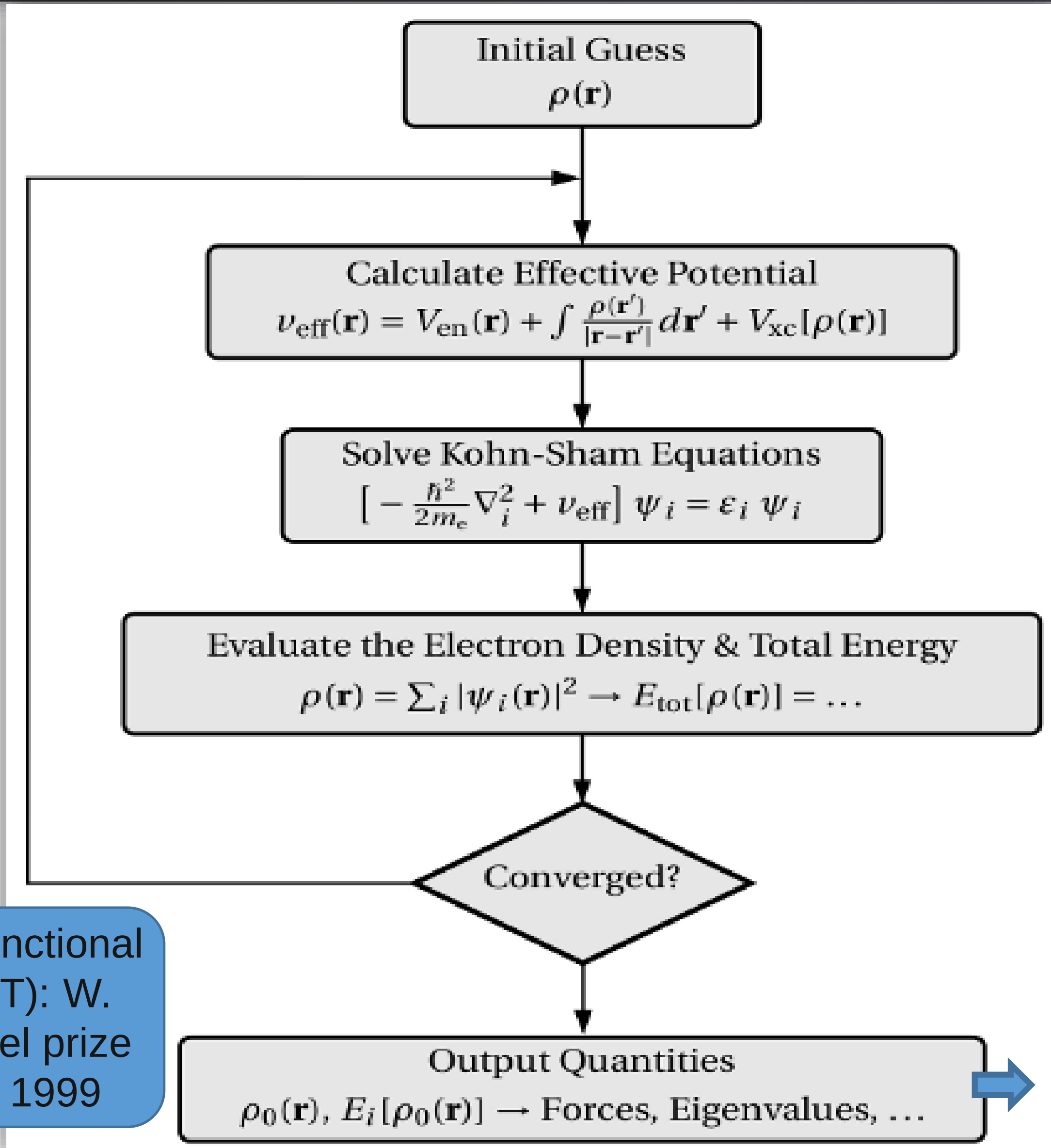
1.Use ab-initio tools to relax the geometry of chosen material, obtain their structural, elastic and electronic properties.

2.The relaxed geometries are used in McStas, the neutron scattering simulation code for beamlines, to understand different peaks in the signal, depending on the sample, and beamline description.

3.Correlate ‘micro atomistic scenario’ among a manifold of possibilities to reproduce the observed ‘experimental macro features’.

How ab-initio method works?

ASE



- ✓ Quantum espresso (free)
- ✓ Octopus (free)
- ✓ VASP (licensed)
- ✓ Siesta (free)

TDDFT for excited state properties and dynamics.

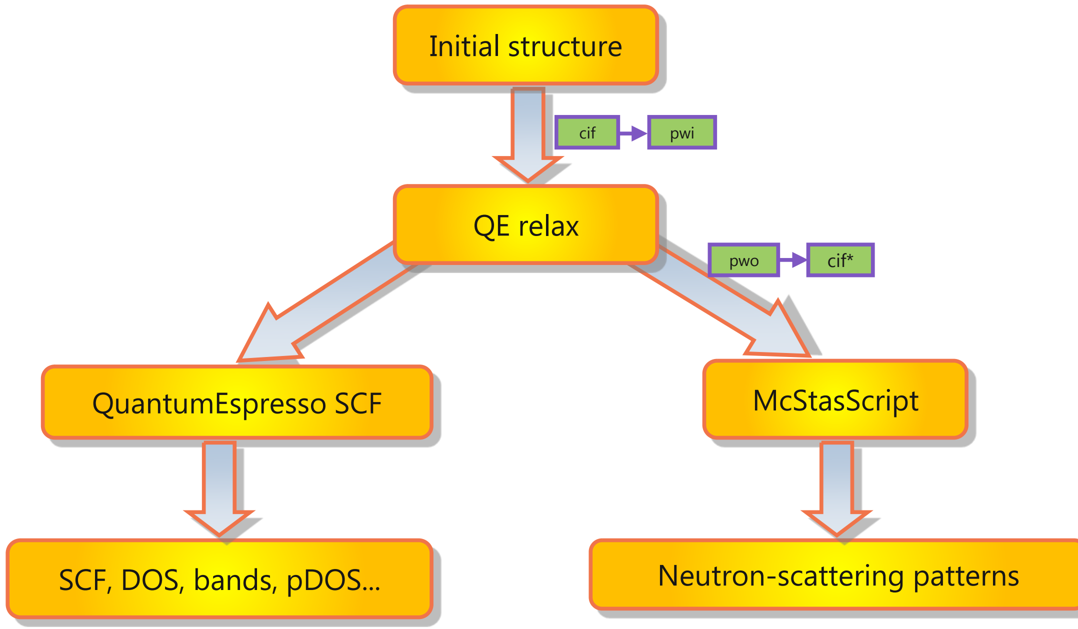
fundamental variable is the many-body charge density.

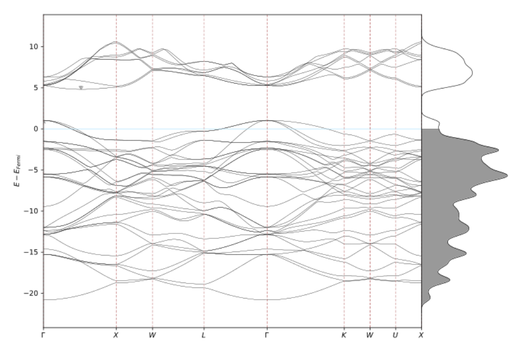
- ➢ Structure, energetics….
- ➢ Cheap, virtual experiment

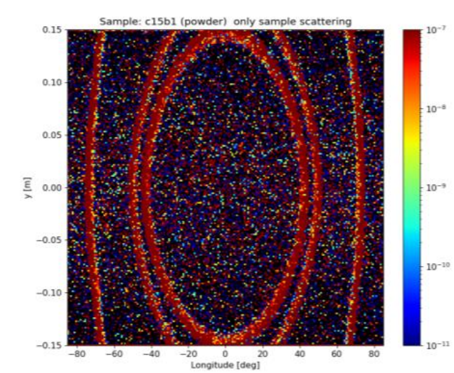
Density Functional Theory(DFT): W. Kohn, Nobel prize Chemistry, 1999

DFT and neutron diffraction of boro-carbon systems

- **Combine and integrate** DFT/TDDFT tools with experiment simulation tools
- Similar idea with ultrafast laser beamline simulations
- Virtual experiments on accurately simulated materials
- Aim: development of a single API environment in Python:
  - QE (and more): **AES**;
  - McStas: **McStasScript**;
  - **SimEx**



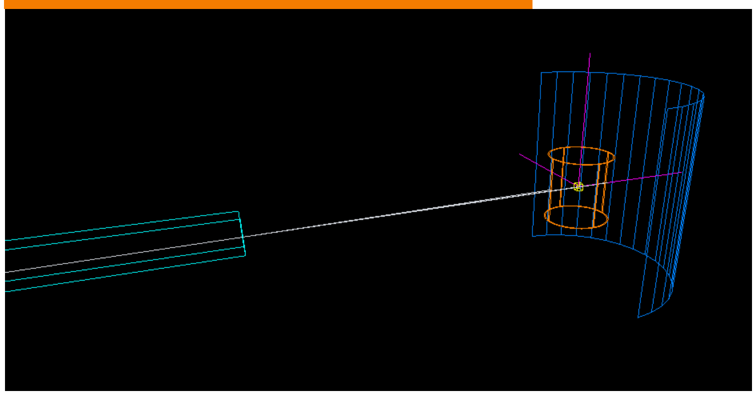




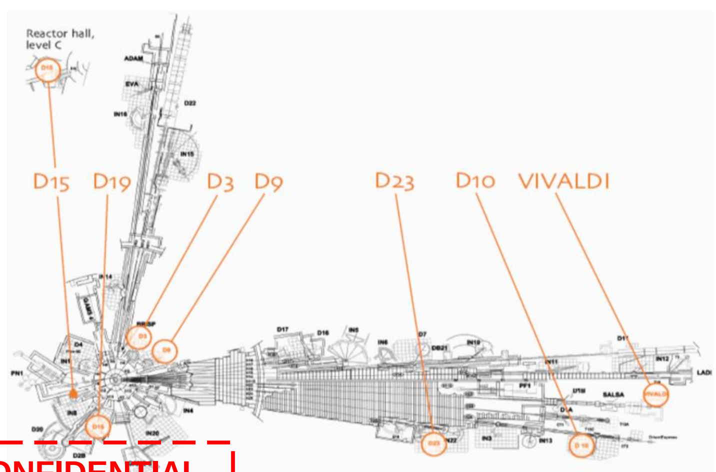
DFT and neutron diffraction of boro-carbon systems

Simulation of neutron scattering beamlines

VIVALDI, ILL, France

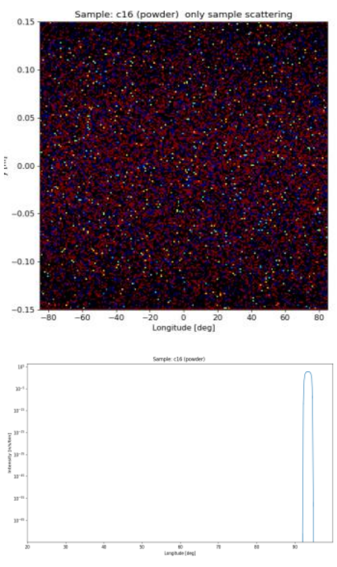


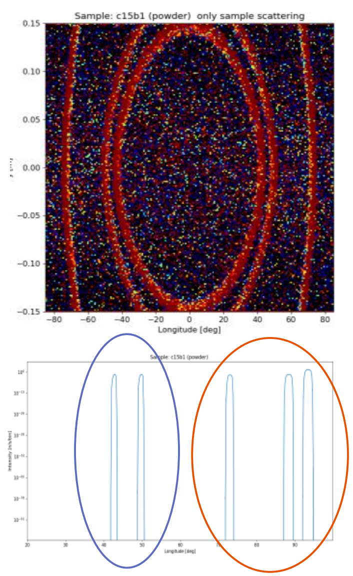
DMC, PSI

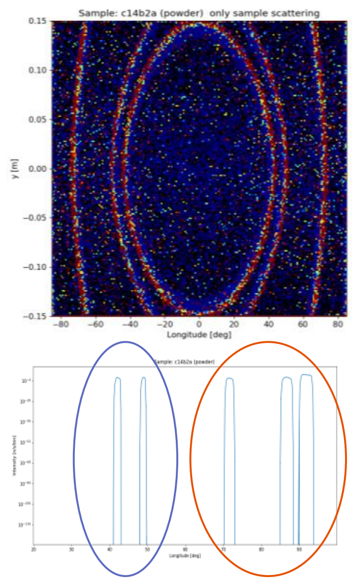


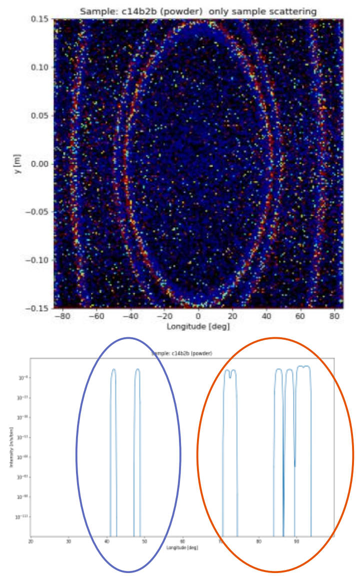
CONFIDENTIAL

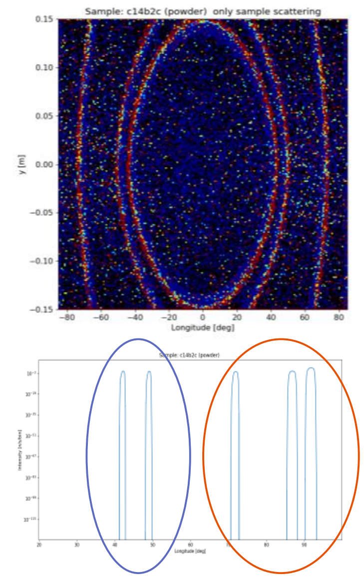
Simulation for neutron scattering using chosen beamlines set-up with McStas











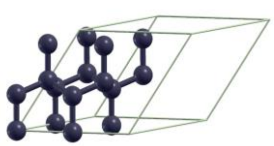
C16

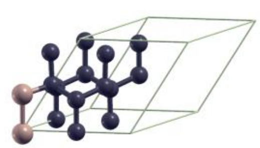
C15 B1

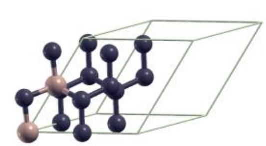
C14 B2 - a

C14 B2 - b

C14 B2 - c

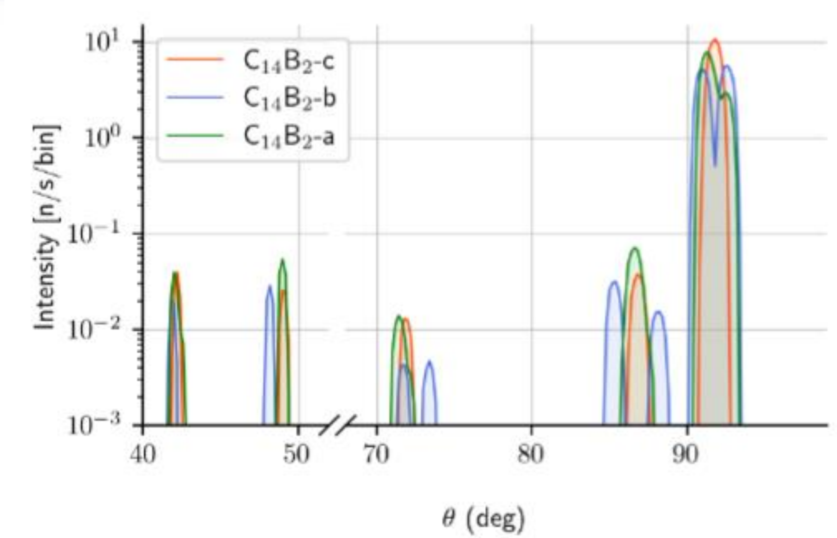


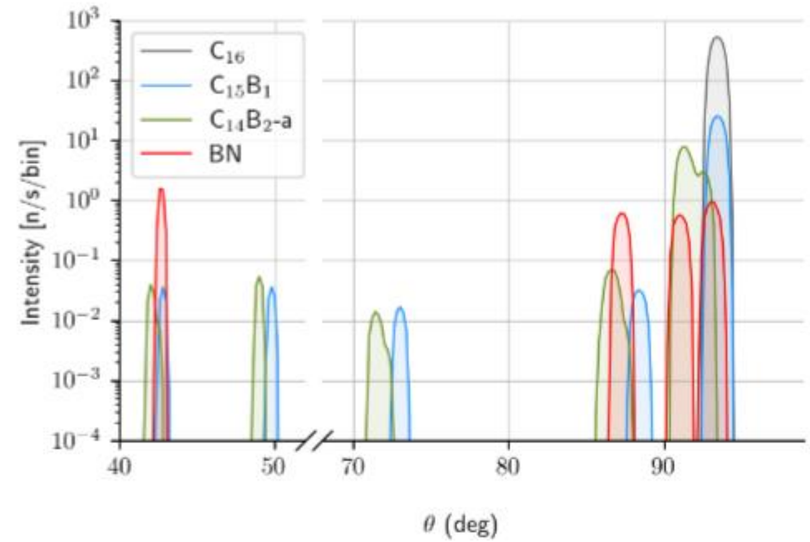




Total signal of VIVALDI:	6.6 % of C16	4.3 % of C16	3.1 % of C16	6.1 % of C16

Understand different peaks in the signal, depending on the sample…….. Correlating with experimental features….





Why is this important?

- ✓ Correlating the atomic-scale micro-scenario', among a manifold of possibilities, to the experimentally observed 'macro-features', by beamline simulation
- ✓ **Similar 'analysis protocol', approach can be envisioned for complete ultrafast laser beamline, as in facilities like ELI.**
- ✓ **The 'combinatorial simulation approach' to support user experiment** has potential for all EU laser/beamline facilities.

What do we achieve with Start-to-End simulation platform?

An efficient, high-fidelity and simple-to-use simulation platform?

- Narrowing the range of parameter space according to phenomena of scientific interest.
- Investigating the feasibility of measuring signal (some degree of confidence).
- Informing optimal design of instrumentation for future experiment stations.
- Probing physical understanding of experimental observations.
- Generating simulated data sets for initial training of Machine Learning algorithms (e.g. for wave optimization, 3D structure reconstruction)

Photon source

- Pulse duration, profile, repeatation rate
- Energy,beam wavelength
- Polarization, focussing

Photon propagation

- Beamline optics (lens, mirror, monochromator..) raytracing
- Optics profile, distance
- Focussing of radiation field

Photon-Matter interaction

- Molecular dynamics/ DFT
- Particle-In-Cell
- Radiation-Hydrodynamics

Sample description/trajectory

- Electron structure
- Atom positions
- Density,temperature,pressure

Signal generation and processing

- Scattering/ Absorption/Emission
- Detector noise
- Identify ideal signal conditions

Virtual lab for optimization of user experiments

- How much data is enough?
- What (detrimental) effects can be ameliorated by simply collecting more data?

❖ Efficient scientific data management, connecting EOSC - **PaNOSC + ExPaNDS → …. IMPULSE**

Project Objective

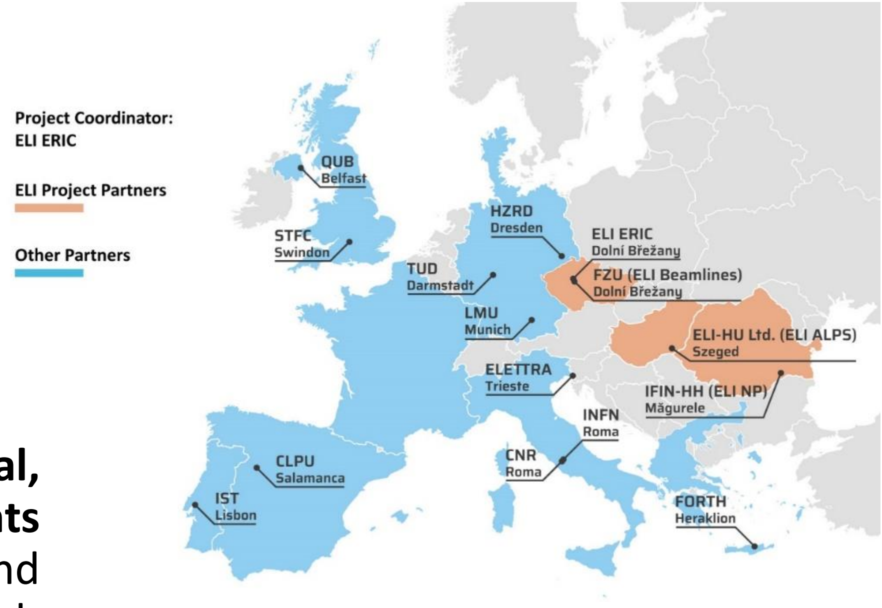
Uniting the ELI facilities and making them **accessible for users through one single, high-quality access point**.

- Develop joint management culture and capabilities of ELI facilities with an efficient use of resources
- Identify opportunities for technical synergies to lower operations costs and increase availability for users
- Scientifically optimize performance and potential of ELI systems to generate interest in ELI and in laser science

IMPULSE addresses the **key scientific, technical, organisational,** and **management requirements** of this transition, **building user communities** and **expanding the ELI member consortium** . Though IMPULSE focuses primarily on ELI, its results will impact all European high-power laser facilities.

- **15 Partners**
- **10 Countries**
- **42 Months**
- **€19.9 Million**

Integrated **M**anagement and o**P**erations for **U**ser-based **L**aser **S**cientific **E**xcellence



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Many thanks to my WP5 colleagues, my ELI colleagues… computation support

To Teodor, Florian, Andy

THANK YOU FOR YOUR ATTENTION!

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