



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

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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

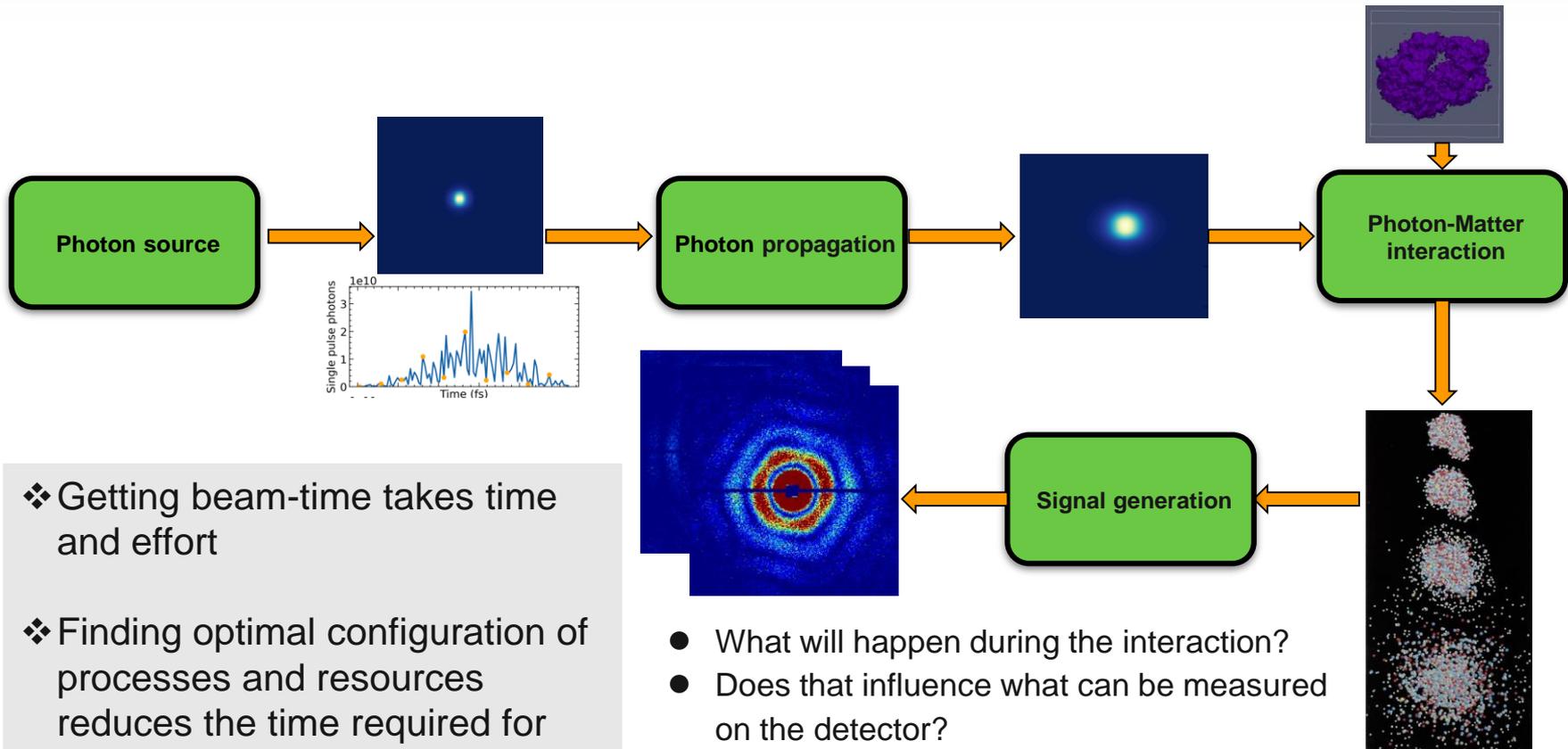


ELI-ALPS Szeged
Hungary
Ultrashort laser pulses at high
repetition rate

<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).

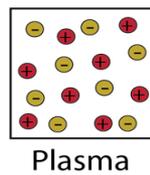
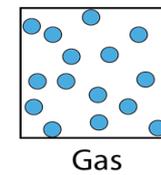
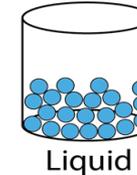
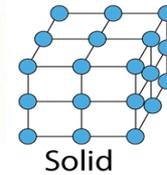
Computation/simulation is used for process analysis and process optimization.

Use LASER to understand and control materials



Periodic Table of the Elements

1 1IA 11A																	18 VIII A 8A	
1 H Hydrogen 1.0079	2 IIA 2A											13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	2 He Helium 4.0026	
3 Li Lithium 6.941	4 Be Beryllium 9.01218											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.0074	8 O Oxygen 15.9994	9 F Fluorine 18.998463	10 Ne Neon 20.1797	
11 Na Sodium 22.98976928	12 Mg Magnesium 24.305	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	VIII 8		9	10	11 IB 1B	12 IIB 2B	13 Al Aluminum 26.9815386	14 Si Silicon 28.0855	15 P Phosphorus 30.973762	16 S Sulfur 32.06	17 Cl Chlorine 35.4527	18 Ar Argon 39.948
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.95591	22 Ti Titanium 47.88	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938	26 Fe Iron 55.847	27 Co Cobalt 58.9332	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.6	33 As Arsenic 74.9216	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.80	
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.9058	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.94	43 Tc Technetium 98.9062	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.9055	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.757	52 Te Tellurium 127.6	53 I Iodine 126.90447	54 Xe Xenon 131.29	
55 Cs Cesium 132.90545	56 Ba Barium 137.327	57-71 Lanthanide Series	72 Hf Hafnium 178.48	73 Ta Tantalum 180.9478	74 W Tungsten 183.85	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.084	79 Au Gold 196.96657	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.98039	84 Po Polonium [209]	85 At Astatine [222]	86 Rn Radon [222]	
87 Fr Francium [223]	88 Ra Radium [226]	89-103 Actinide Series	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [271]	111 Rg Roentgenium [272]	112 Cn Copernicium [285]	113 Uut Ununtrium [288]	114 Fl Flerovium [289]	115 Uup Ununpentium [288]	116 Lv Livermorium [293]	117 Uus Ununseptium [294]	118 Uuo Ununoctium [294]	
		57 La Lanthanum 138.905	58 Ce Cerium 140.116	59 Pr Praseodymium 140.90766	60 Nd Neodymium 144.24	61 Pm Promethium [144.9127]	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92534	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93032	68 Er Erbium 167.26	69 Tm Thulium 168.93481	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967		
		89 Ac Actinium [227]	90 Th Thorium [232]	91 Pa Protactinium [231]	92 U Uranium [238]	93 Np Neptunium [237]	94 Pu Plutonium [244]	95 Am Americium [243]	96 Cm Curium [247]	97 Bk Berkelium [247]	98 Cf Californium [251]	99 Es Einsteinium [252]	100 Fm Fermium [257]	101 Md Mendelevium [258]	102 No Nobelium [259]	103 Lr Lawrencium [260]		
		Alkali Metals	Alkaline Earths	Transition Metals	Basic Metals	Semi-Metals	Nonmetals	Halogens	Noble Gases	Lanthanides	Actinides							



→ Add Heat

Control and trace the motion of atoms in molecules

⇒ Control chemical reactions

Control & trace electrons inside atoms & molecules

Femto

Atto

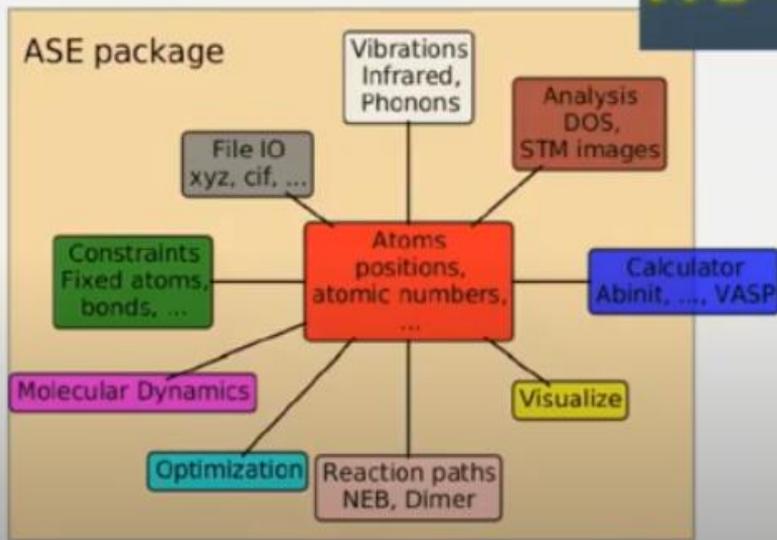


Within WP5 – combine ASE and McStas

Atomistic simulation environment (ASE) for Density functional study

Atomic simulation environment

A Python library for working with atoms



Aim: Unified interface

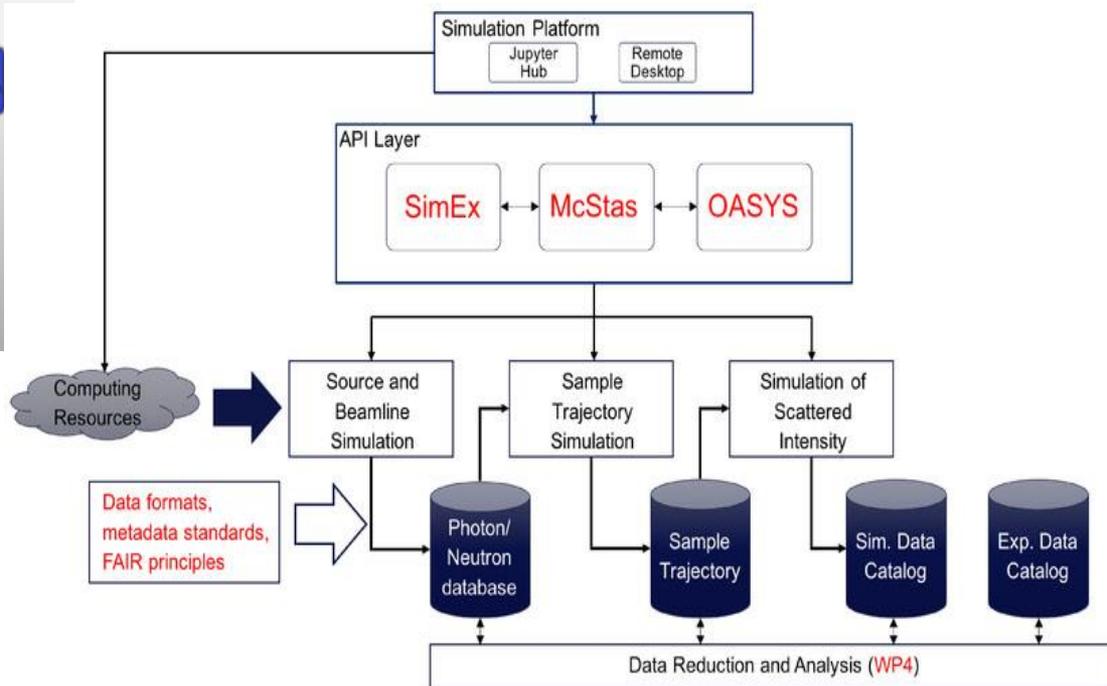
SimEx: flexible modular code to mimic an entire laser beamline.

McStas: Neutron beamlines

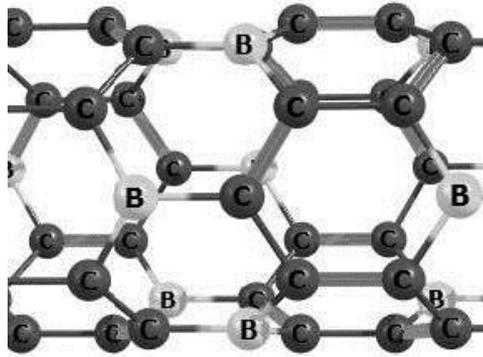
IMP: Interaction with materials

<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

- ❖ Current use case- ASE + McStas - using a common platform
- ❖ FAIR Data Management -> relates to ExPaNDs, IMPULSE

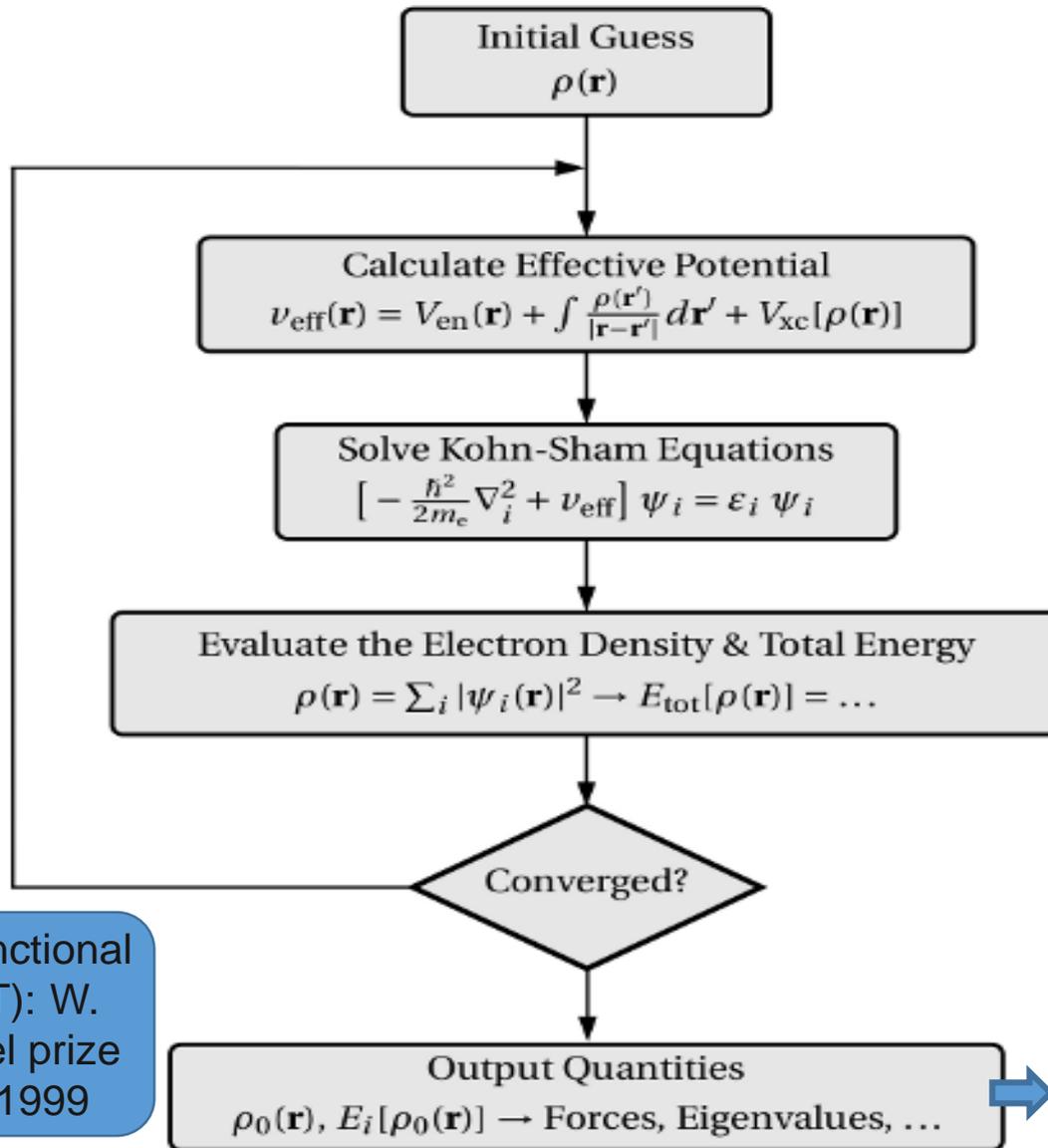
Use Case Action Flow

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



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

- ✓ 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....

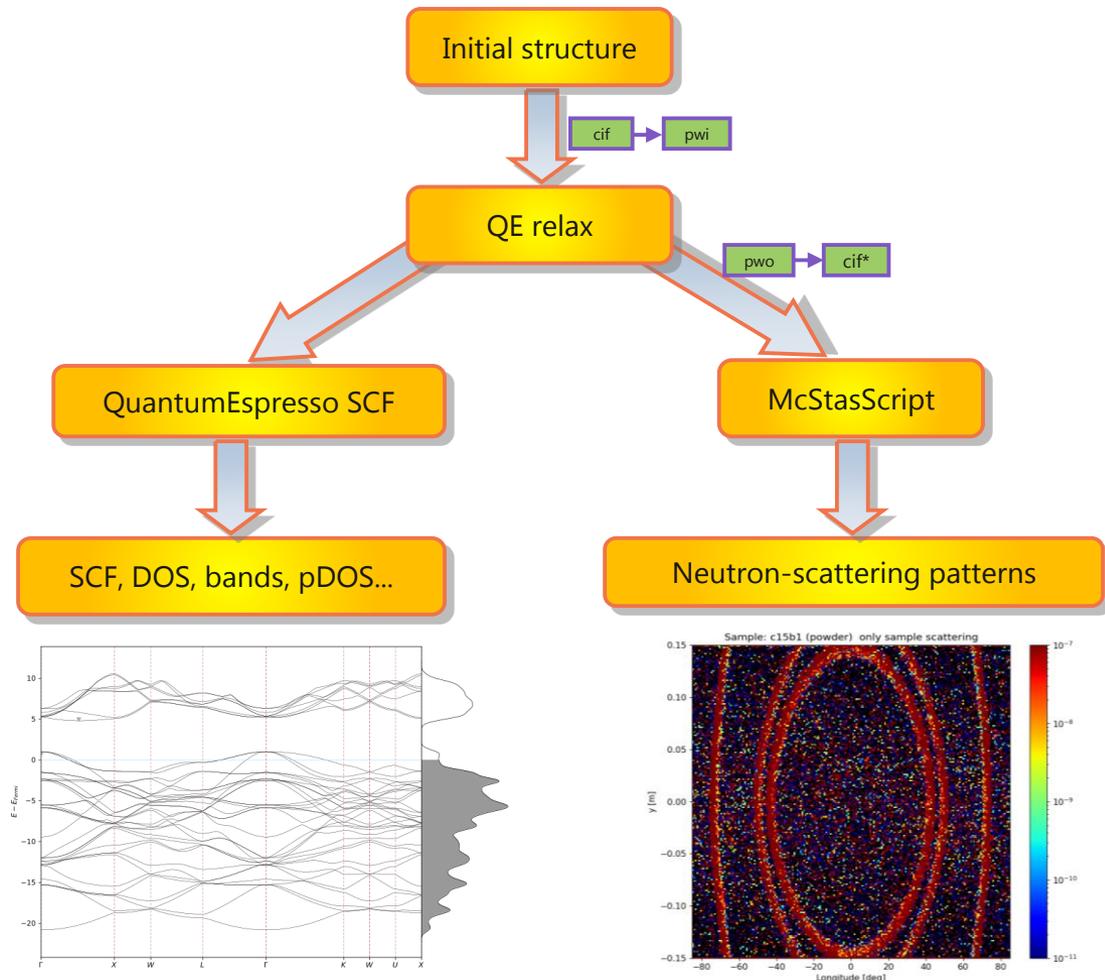
➤ Cheap, virtual experiment

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**

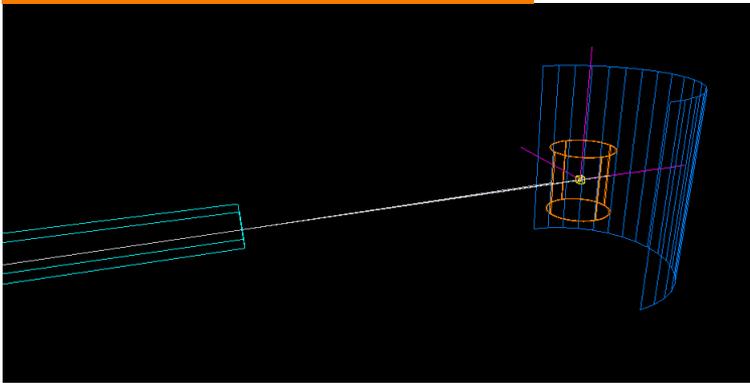


DFT and neutron diffraction of boro-carbon systems

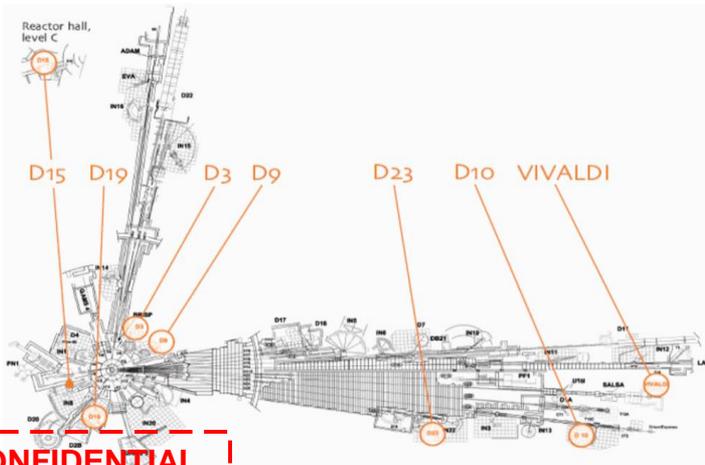
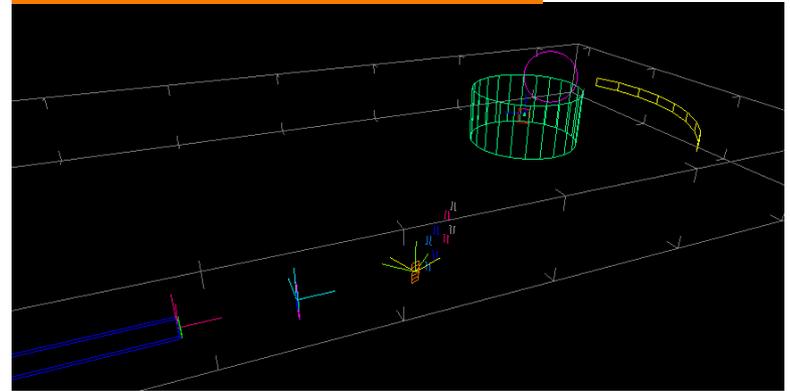


Simulation of neutron scattering beamlines

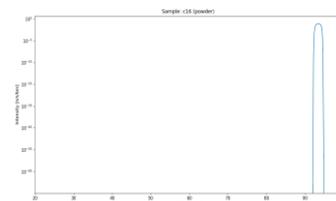
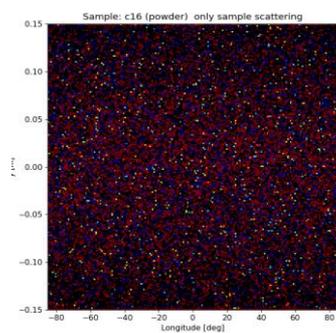
VIVALDI, ILL, France



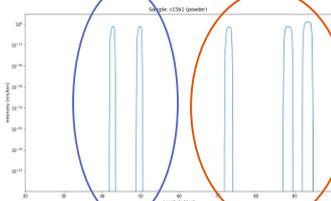
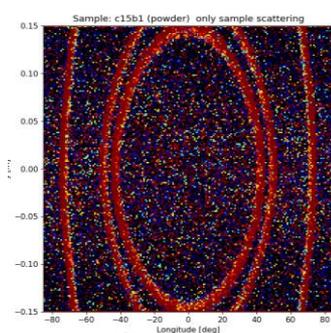
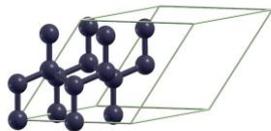
DMC, PSI



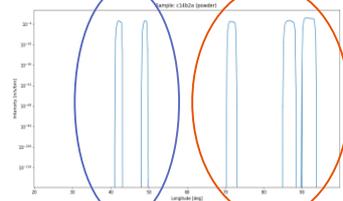
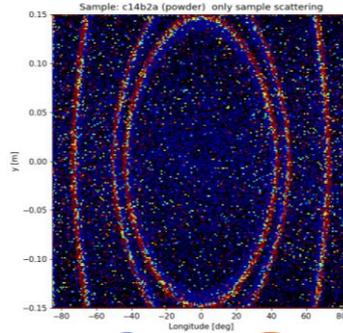
Simulation for neutron scattering using chosen beamlines set-up with McStas



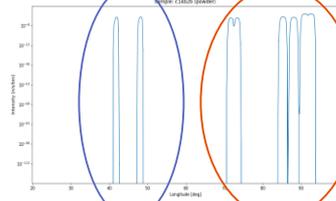
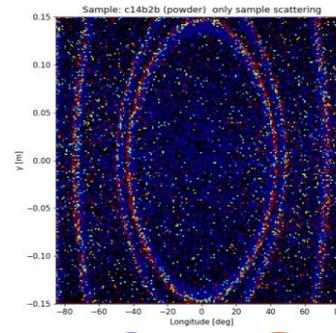
C16



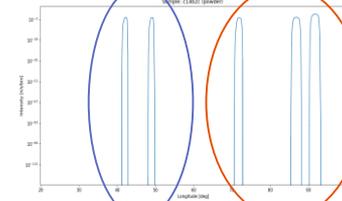
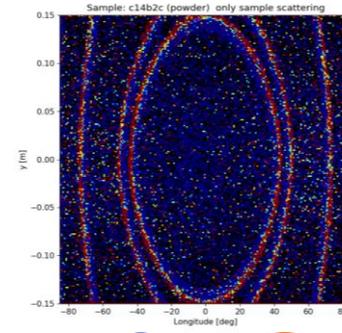
C15 B1



C14 B2 - a



C14 B2 - b



C14 B2 - c



Total signal
of VIVALDI:

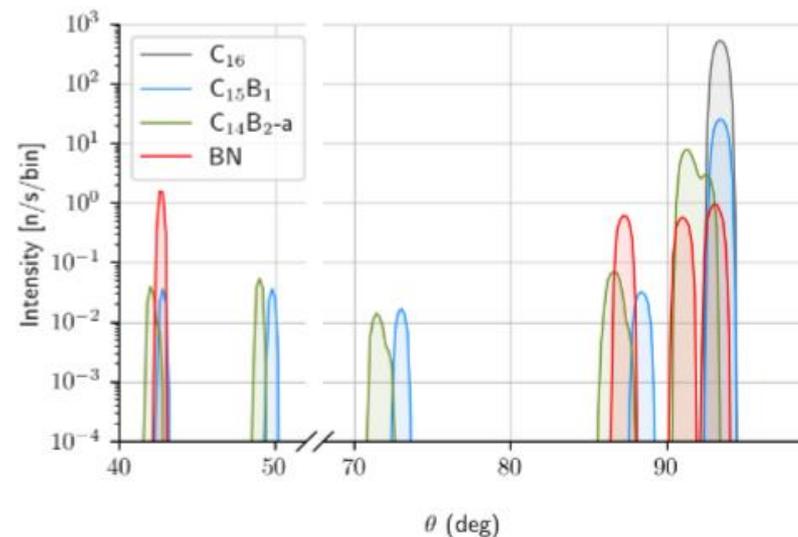
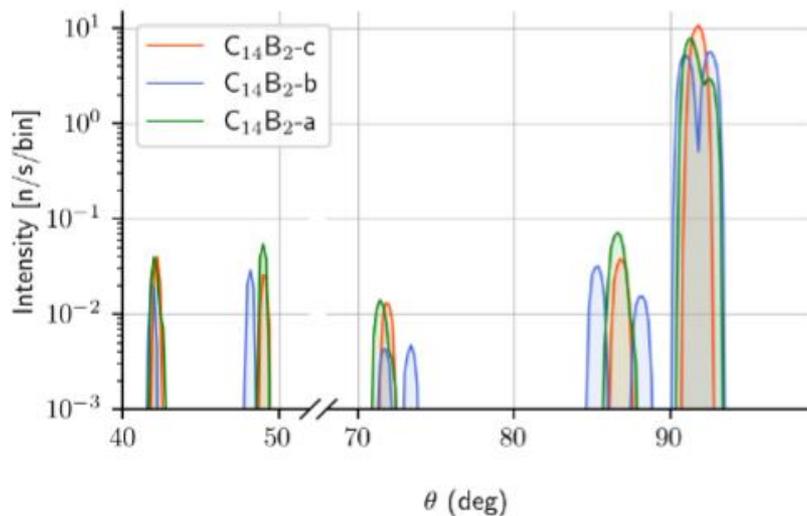
6.6 % of C16

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, repetition 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

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

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

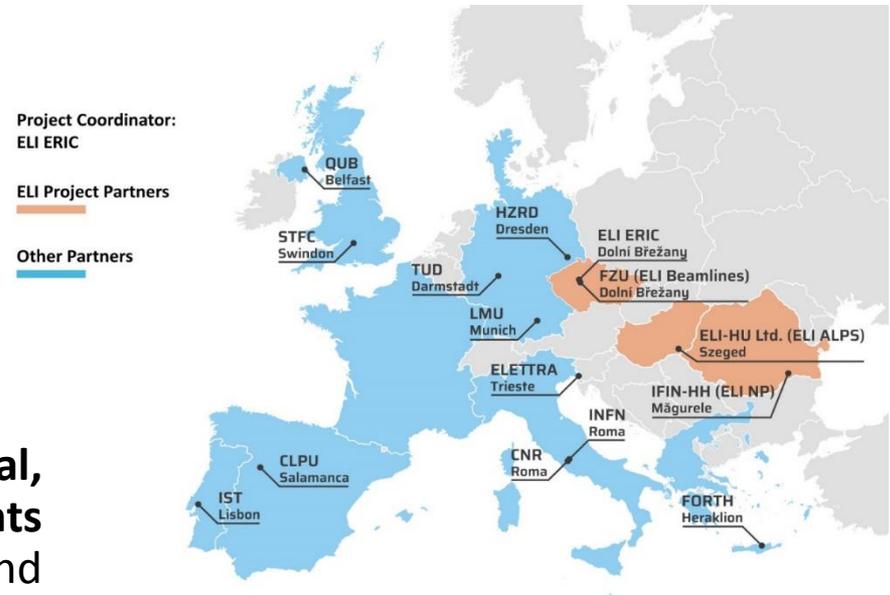
Uniting the ELI facilities and making them accessible for users through one single, high-quality access point.

- 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 Management and Operations for User-based Laser Scientific Excellence



IMPULSE is funded by the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871161

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



To Teodor, Florian, Andy

THANK YOU FOR YOUR
ATTENTION!

SZÉCHENYI 2020



HUNGARIAN
GOVERNMENT

European Union
European Regional
Development Fund



INVESTING IN YOUR FUTURE