WG1.2 Possible topics for HE-INFRA-2024-TECH-01-01 call

Idea1 "Supercurve"

Building on LEAPS Innov Superflat: we would propose a similar PCP type action to develop industrial techniques for processing strongly curved, aspheric and freeform optics with sub-50 nrad rms slope errors and sub-1nm peak-to-valley shape errors.

Idea2 Optics contamination mitigation and coating degradation

High value optics generally degrade under X-ray beam exposure. This is a particular problem for reflective optics used with both hard and soft X-ray sources. Degradation mechanisms may be related to progressive contamination of the reflective surface or to evolution/damage of a functional coating. For the former the usually inhomogeneous carbonaceous films which are formed, degrade the optical reflectivity but also create perturbations in the reflected wavefront which progressively degrade the focusing performance of the optics. For the latter, the causes are more diverse but similarly problematic. Eventually these phenomena require the reconditioning (re-coating, re-polishing) or even replacement of the optics. Increased photon flux densities and the desire to exploit the coherent nature of the X-ray beam means that the useful lifetime of optics before intervention is necessary become shorter with the new DLSR and FEL sources. This project seeks to investigate the mechanisms leading to the degradation, and to develop mitigation and remediation methods which can be applied for our user facilities to protect the investment in these valuable optics.

Idea3 Wavefront correction

X-ray beamlines typically employ a reconfigurable array of diffraction crystals and reflective mirrors to efficiently monochromate and transport the photons to the sample under test. However, fabrication errors and misalignment of the X-ray optics leads to deformation of the wavefront, which prevents diffraction-limited imaging of the source. Rather than replacing all optics with state-of-the-art quality, a cost-effective and less-disruptive method to correct wavefront aberrations is the addition of a compensator optic (analogous to eye-glasses to correct human vision). A recent innovation to extend this concept is the use of dynamic compensator optics. Such optics can achieve "active" (quasi-static) or "adaptive" (real-time) compensation of the X-ray wavefront using refractive correctors [1] or deformable X-ray mirrors [2]. Aside from achieving near-perfect optical performance using imperfect beamline optics, such solutions can also purposefully create non-Gaussian X-ray beams, such as a flat-top or split peaks. Measurement and correction of X-ray wavefronts is a hot topic, but existing systems are not straightforward to implement. This project would develop the technology to enable automatic optimisation and control of the X-ray wavefront to benefit a wide range of scientific communities.

[1] "Adaptable refractive correctors for x-ray optics", D. Laundy et al, Optica, 6, Issue 12, pp. 1484-1490 (2019) https://doi.org/10.1364/OPTICA.6.001484

[2] "Fast shaping control of x-ray beams using a closed-loop adaptive bimorph deformable mirror", S. G. Alcock et al, Optica (2023)

Idea4 Spatial diagnostics to optimize FEL/synchrotron performance WG1.4

4.1: Destructive X-ray beam viewer (ESRF, who else?)

Motivation :

Making available (ultimately commercially, off-the-shelve) a low-cost, reliable, compact and well-defined instrument, that is fully optimized to image the X-ray beam-passage and so to provide clear information on the transverse beam-position and also beam-size & profile.
The instrument has standard interfaces & control, both for vacuum, mechanics, translation-control and camera-array read-out. It also comprises survey monument(s) for precise positioning & survey, Its total size/volume/encumbrance would be miniaturized so that it can easily fit in many environments. It aims to have outside dimensions of typically 20x20x20cm.

4.2: Diamond sensor development (EuXFEL, (DIAMOND) who else?)

No commercial supplier for XFELs, challenge to measure at MHz, device, material and electronics development is required. Demonstration required on device lifetime

Non-invasive position and intensity measurements in particular also at high (MHz) rates for hard X-rays can be provided by sensors based on electronic grade single crystal CVD diamond. In particular, at very hard X-rays the gas-based devices lose sensitivity and diamond-based sensors are a useful complement. They can provide pulse-resolved intensity and beam position measurements, in average for synchrotrons but also at high rates for FELs. Commercial devices are available for synchrotrons but not for FELs. For synchrotrons additional some modest spatial resolution would be important. At FELs these sensors can fill the capability gap beam position measurements at rates *higher than* 10 - 100 Hz.

4.3: Spatial coherence monitor/wave front sensing (ALBA, who else?)

Motivation:

This project aims to develop a novel sensor to measure the two-dimensional transverse coherence length of the X-ray part of the Synchrotron Radiation (SR) produced in particle accelerators. This sensor not only provides the SR coherence size, but also the two-dimensional transverse particle beam size: this makes it especially valuable for both beamline scientists and accelerator scientists, and it also of interest for both Synchrotron Light Sources (SLS) and Free Electron Lasers (FELs).

Particle beam dimensions tend to become smaller, reaching um or sub-um range in the future Low Emittance Accelerators. Thus, direct imaging techniques are limited by diffraction-related effects, and become no longer suited to measure such small beams. Instead, this method avoids this limitation as it is based on coherence measurements.

Idea5: Advanced codes/AI/Virtual diagnostics

Key to capitalize on high rep rate FEL sources

5.1: Improve data fidelity(DESY, EuXFEL?, who else?)

Using AI to improve data fidelity from signal to noise limited detectors.Train AI on a combination of a high-resolution invasive spectrometer and lower-resolution online spectrometer to improve the spectral resolution of the non-invasive spectrometer when the invasive spectrometer is removed during beam delivery to the experiment. Compensate partially broken/missing detector information by trained AI.

5.2: Automated focal spot alignment and maintenance(FLASH, FERMI, EuXFEL, who else?)

Critical for routine investigation of nonlinear X-ray science

Automated codes couple with wavefront/spatial sensor to align KB or similar mirror systems or CRL lenses to a predetermined focal spot size and 3D position

- Combined with wavefront sensor for online feedback
- Speedup initial setup and focus size and position characterization
- Characterization needed with full beam power in some situations
- Automated codes couple with virtual foci to maintain exact spatial overlap of X-ray and laser foci at predetermined 3D position. Automated codes maintain overlap of photon beam to online diagnostics, in particular in 24/7 automatic operation.
- Codes for feedback for optics and to feedback beam trajectory

Idea6: X-ray and laser arrival time probes(PSI, EuXFEL, who else?) WG1.4

Key requirement for following site specific charge transfer processes (energy)

Even after state of the art stabilization there remains a temporal jitter between the arrival time of X-ray pulse and laser pulses used in time resolved measurements at all FEL and time resolved synchrotron facilities in the world. This uncertainty between the exact timing between the two pulses results in a limitation of the time resolution achievable for measurements at these facilities, which is in many cases larger than that achievable from the ultrashort laser and X-ray pulses routinely available.

X-ray and laser cross correlation diagnostics have been built at most facilities routinely called time tools. Their fundamental resolution has been demonstrated to be sub 20 fs, but this has not translated into routine ultrafast time resolutions being achievable by the regular user of FEL facilities. Of critical importance here is the current cross correlation tools and generally separated by some meters from the experiment interaction point and use different laser beam paths. Residue drifts and uncorrelated jitter between the experiment interaction and cross correlation are not accounted for

Proposed here is a simple and easily applicable combination of timing probes which independently measure the X-ray and laser arrival time to a universal reference with a high degree of accuracy.

Idea7: Online single-shot temporal profile diagnostics (DESY, EuXFEL, HZDR, INFN,who else?)

: The upcoming prospects of attosecond XUV and X-ray pulses, also in combination with polarization control, allow to tackle fundamental questions of ultrafast charge-migration dynamics in (chiral) molecular systems with full site-specificity, eventually even in the liquid phase.

Highly nonlinear and ultrafast processes e.g. in molecules can provide new insight into the complete picture of the role of Coulomb potentials, their attosecond evolution and its impact on phenomena of (stereo)chemical evolution via electron spectroscopy. Based on intense, circularly polarized X-ray pulses from FELs with detailed knowledge of the attosecond time–energy structure, a novel perspective for investigating charge-migration dynamics in e.g. chiral molecules on an attosecond time scale arises, which will attract new interdisciplinary teams of users to FEL science.

In fact, a broad variety of experiments depends crucially on the precise and prompt knowledge of the actual pulse duration and/or pulse structure. This holds true not only for resonance spectroscopy of, e. g., transient systems, but also for the bulk of ultrafast investigations of electronic and nuclear motion within molecules and solids at FELs. In this regard, angular streaking has been demonstrated to be a unique tool for characterizing free-electron laser pulses at the attosecond frontier (1,2). It has originated and leveraged a new field of scientific access at FELs that currently gains accelerated interest all over the world.

Since many FELs in the world have started or envision to push forward into the attosecond pulse duration regime (also in combination with polarization control), it is an urgent goal to not only demonstrate the capability of attosecond-resolved pulse characterization, but to evolve it into a robust pulse diagnostic method that can give real-time feedback to the machine as well as to users. In a further step, this diagnostic methodology is determined to not only give feedback but also to directly interact with the machine operation. Both the online pulse reconstruction and the machine interaction will be based on AI-methods such as autoencoders and convolutional neural networks (3).

Application of these techniques in the hard x-ray domain (few keV to several 10 keV) require advances in the hardware implementation (4).

1) N. Hartmann *et al.*, *Nat. Photonics*. **12**, 215–220 (2018)

2) R. Heider *et al.*, *Phys. Rev. A*. **100**, 053420 (2019)

3) K. Dingel *et al.* Scientific Reports **12**:17809 (2022)

4) J. Laksman *et al*., Rev. Sci. Instrum. 93 (11), 115111 (2022)

M.Calvi Wednesday, 21 December 2022

Dear Michele,

Here after the list of the topics which could be of interest for the next HE-INFRA-2024-TECH-01-01 call. As you suggested, for this first round we (WG2) are just proposing all subjects which are under debate without evaluating the coherence of the whole proposal and without any internal ranking. In January, we will meet and refine the list taking into account the feedback of the RDB. Please consider the formulation of the topics as a tentative draft useful only to give a brief idea of the subject and nothing more.

1. **Idea 8 PermaLIC 2.0** (Suitable as well for the Green deal?) (F. Perez, ALBA)

   The goal of the proposal is two-fold, from one side, to produce prototypes which would validate the techniques required for producing accelerator magnets in series. Which shall comply with the required magnetic quality specifications, including long term stability, and which shall have built-in tunability to cope with the required flexibility for error correction. On the other hand, to establish the methodology to produce magnets out of recycled material, and validate the process with a “green magnet” prototype.

2. **Idea9 HarmonLIP** (P. F. Tavares, MAXIV)

   For future light sources aiming to achieve even lower emittances than the present suite of existing and planned sources, good control of the bunch length will be even more critical and one may envisage the need to achieve considerably larger lengthening ratios than those achieved today (which vary from 2 to 5). Combining different harmonic systems may be a mechanism to provide such extremely long bunches and this project aims to experimentally demonstrate its feasibility.

3. **Idea10 HighBri** - High Brightness (complementary to HarmonLIP) (M. Calvi, PSI)

   Applications of High Temperature Superconductors (HTS) REBCO tapes and bulks to increase the brightness of next generation beamlines. The performance of super-bends, wigglers and undulators will be greatly enhanced by this new and challenging technology and REBCO will find a new and attractive application which will contribute to its development.

4. **Idea11 ARA** - Androids for Remote Access (R. Wanzenberg, DESY)

   Androids can access parts of the facility normally forbidden to people due, e.g., to radiation hazards in accelerator bunkers, and they can be the eyes and the hands of a human operator. The collaboration with universities and research institutes, especially CERN, will complement the business relation with the involved procurement companies. The android can be remotely operated by a human who guides each of its actions using enhanced/virtual reality tools. This could be the initial mode of operating them within our facilities. If this approach would be demonstrated successful, a higher degree of automation could be evaluated. This step requires the implementation of machine learning algorithms for pattern recognitions to information than conventional methods such as images from beam position monitors, screens or transverse deflectors. Such models could also allow to understand and overcome the resolution limit, as well as to extract beam properties for machines and locations where conventional diagnostics may not be available. They promise computational efficiency in otherwise intensive processing for extracting meaningful information, as well as enable continuous effective mixed training using both models and observational machine data. Non-destructive diagnostics also allow for monitoring and optimization of the machine properties for the specific experiment taking place.

6. Idea12 **LPS** - Longitudinal Phase Space (Simone-Sverker-Pavel)
   Longitudinal Phase Space e-beam physics for fully coherent FELs and high-field THz pump sources. An injector test facility with the suitable characteristics and requiring minor modifications shall be identified (MAXIV, PSI?) to conduct an experimental campaign to demonstrate these new concepts.

Idea13 Compact EUV/soft x-ray spectrometer with polarization analysis

Laura Foglia[1], Filippo Bencivenga[1], Martin Beye[2], Majed Chergui[3]

1. Elettra Sincrotrone Trieste S.C.p.A, Trieste, IT.
2. Deutsches Elektronen-Synchrotron: Hamburg, Hamburg, DE
3. Ecole Polytechnique Fédérale de Lausanne

For several years now, society has struggled to keep the balance between productivity and sustainability. The challenges we have faced in the last years (including pandemics, energetical crisis, lack of raw materials and climate change) have stressed the need of reducing the overall environmental costs of our lifestyle. Clean energy production and storage, bridging the digital divide between first and third world countries with efficient and low-cost computing and data storage, clean water and sanitation, catalysis and decarbonization, targeted drugs, are all societal challenges that can be tackled with help of x-ray-based fundamental research. Nevertheless, this calls for radically new approaches both from the technological as well as fundamental science point of view. This, in turn, means the need for substantial advances in experimental methods and instrumentation, which are nowadays often at their resolution limits. In particular, the deep understanding of many of the systems which are devised as forefront technology, such as complex magnetic systems, chiral molecules, polar metals, require the capability of measuring small signals with energy and polarization analysis under flexible directions, vacuum, spatial resolution and strong background suppression.
This work package aims at developing a compact soft x-ray spectro-polarimeter with applications at K-edges of light elements and L-edges of 3d transition metals, thus covering a wide range of biologically interesting samples and strongly correlated materials. As depicted in the figure, this setup combines: i) x-ray diffraction optical elements (XDOEs) for low resolution spectral analysis, ii) multilayer (ML) mirrors at the Brewster angle (≈45° incidence) for polarization analysis, background/stray light rejection and flexible tuning to match the signal frequencies of interest by tweaking the angle of incidence (ϕ) on the ML; and finally iii) soft X-ray detectors with high sensitivity, down to single-photon. The use of two MLs permits parallel detection of both polarization components of the selected signal beam(s), while the beam transmitted from the XDOE can be detected by a photodiode and used for in-situ normalization. Moreover, two XSPs can be used to detect transmitted and reflected signals in parallel. We envision standard and compact in-vacuum mechanics, representing the core of the instrumentation, as well as standard interfaces, which facilitate implementation/replication at partner institutions. XDOEs and MLs are realized on standard supports (to be easily integrated in the mechanics) and designed for a given set of experiments. Depending on the application, one may devise a set of XDOEs and MLs that can be flexibly changed (on-line) during the experiment. This project will benefit the partners of the consortium and, more in general, scientific and technological stakeholders of the European Union under several aspects. First, this instrument is based on new devices and processes, which will be developed within the project and are not necessarily related to the specific application, i.e.: soft x-ray ML coatings, XDOEs and detectors. Moreover, the XSP is devised as portable, to enable experiments at all partner facilities. In this context, we will make all necessary efforts to provide a "seed" for a foreseeable (and convenient) standardization process of instrumentation and protocols at large scale synchrotron, FEL and laser facilities within the consortium.

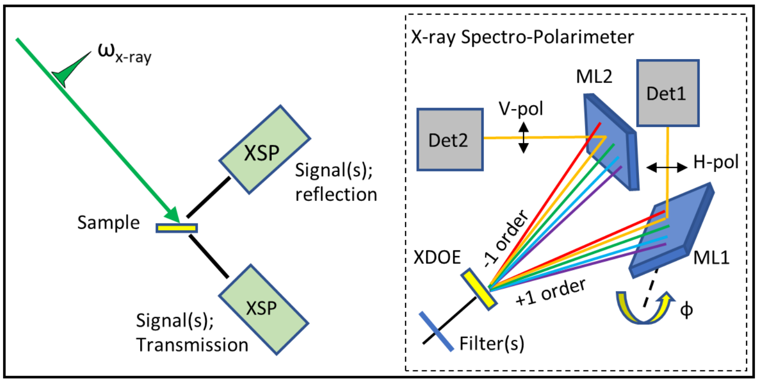

Figure 1 sketches the experimental scheme, where the soft x-ray spectro-polarimeter (XSP - sketched in the hatched area) is used to detect the signals with spectral and polarization analysis; see text for the description of the setup.

HE-INFRA-2024-TECH-01-01 WP proposal:

Idea14 Ion traps for biomolecules and nanotargets

- Interested LEAPS partners: DESY (Markus Gühr et al.), FELIX (Britta Redlich et al.), SOLEIL (John Bozek et al.)
- Potential additional LEAPS partners: ELETTRA, HZB, MAX IV, …
- Potential university partners: Uni Groningen (T.A. Schlathölter, R. Hoeckstra et al.), …
- Potential industry partners: equipment development for ion traps (e.g. Fasmatech, MS Vision, Bruker …)

Expected impacts:

- Life science
- Nanoparticles within energy/catalysis research

Expected outcomes:

- Strengthen community across LEAPS
- Bring together THz and X-ray community
- Joint data standards
- Drive instrumentation across synchrotrons and FELs