

#### **EUCALL**

### The European Cluster of Advanced Laser Light Sources

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Work Package 3 – Synergy of Advanced Light Sources

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Joint foresight topics for lasers and FELs in Europe

Lead Beneficiary: ELI

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Deliverable Type	
R = Report	R
DEM = Demonstrator, pilot, prototype, plan designs	
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Dissemination Level	
PU = Public, fully open, e.g. web	PU
CO = Confidential, restricted under conditions set out in Model Grant Agreement	
CI = Classified, information as referred to in Commission Decision 2001/844/EC	































# **Contents**

1.	Introduction	3
2.	Addressing Societal Challenges Using Advanced Laser Light Sources	5
3.	Building a Targetry Network for High-Repetition Rate, High-Power Laser Facilities	14
4.	Theory and Simulation of Photon-Matter Interaction	21
5.	Future Strategies for Research Infrastructure Operation	34
6.	Conclusions, recommendations and future activities	40
	6.1 Addressing Societal Challenges Using Advanced Laser Light Sources	40
	6.2 Building a Targetry Network for High-Repetition Rate, High-Power Laser Facilities	40
	6.3 Theory and Simulation of Photon-Matter Interaction	41
	6.4 Future Strategies for Research Infrastructure Operation	41
7.	Summary and Outlook	42



# 1. Introduction

One of EUCALL's primary objectives is the identification of joint foresight topics in science and research policy with the desired outcome of further strengthening the portfolio of advanced laser light sources in Europe. Within EUCALL WP3, foresight topics were identified and presented to the Steering Committee, Executive Board and to the Scientific Advisory Committee (SAC). The latter was especially active in recommending further development of the joint foresight topics. Each topic sets up a vision for a future activity of the advanced laser light source communities, parts thereof or new alliances among the advanced laser light source communities with new outside communities. For each foresight topic, workshops were organized at which invited and contributed presentations on relevant topics, from within and outside EUCALL, elaborated the state-of-the-art, current and future needs. These activities are considered as seeds for future cooperation and collaborations, and are summarized in this report.

A first event addressed urgent societal challenges and how these may be solved making use of the combined properties of laser and x-ray sources. The topics for discussion were Technology and Engineering, Information Technology, Energy, and Health. Keynote speakers presented an overview of key material science challenges for each topic and summarized developments at light source RIs, while further invited speakers presented examples combining experiments at laser light sources. A summary of this event, the outcomes and follow-up activities are presented in Section 2.

A second activity arose from the challenges presented to both users and RI operators from high-repetition-rate, high-power laser experiments, which will soon become possible at facilities such as ELI, ESRF and European XFEL. The provision of adequate targets at sufficient number is a key requirement for the community to make best use of the new research capabilities. A coordinated strategy to provide targets or access target fabrication infrastructures might therefore be needed. Experimental challenges following laser-target interaction involve the protection of the surrounding equipment and optics from debris/shrapnel and electromagnetic pulses, as well as heating and materials activation. Two workshops were organized to address these issues as satellite meetings of EUCALL's 1<sup>st</sup> and 3<sup>rd</sup> Annual Meetings and their outcomes are discussed in Section 3.

Experiments at modern laser light sources provide new capabilities and insights, requiring significant support and advances in theory and modelling for the interpretation of results. Examples are photon-matter interaction, free-electron laser (FEL) source descriptions or complex time-dependent theories to describe systems dynamics, including transition states. There is a clear need for advanced simulations to accompany experiment results. EUCALL organized an open workshop in order to discuss these needs via keynote presentations from invited speakers and contributed presentations from the registered participants. In Section 4 a summary of this activity is provided.





EUCALL's final event aimed to disseminate the results of the "Synergy of Advanced Light Sources" work package (WP3) to its stake-holders and to policy-makers. This workshop focused on the presentation and discussion of strategies, operation needs, and possible frameworks for future collaborations between advanced laser light source research infrastructures, as well as an exhibition of the technical achievements of WPs 4-7. This meeting was held in Brussels and the key messages that were presented at the event are summarized in Section 5. Finally, in Section 6 we summarize the key results of these activities and recommendations for future collaborations between accelerator and optical laser-based light source research infrastructures.



# 2. Addressing Societal Challenges Using Advanced Laser Light Sources

Within the scope of EUCALL's Joint Foresight Topics, a particular objective is the identification of new research opportunities through the combined use of optical lasers and accelerator-based advanced light sources. EUCALL decided on a science-driven approach towards uncovering future scientific applications and to raise awareness in the community of the future possibilities brought about by the new advanced laser light sources. The approach was to identify relevant case studies addressing a number of important research questions (for example artificial photo-synthesis, light-induced phase-transitions, etc.), and to identify how a portfolio of existing sources have been used in the past, as well as how key players in these research fields can imagine the use of advanced laser light sources in the future.

As a step towards achieving this goal, EUCALL organized the workshop "Addressing Societal Challenges using Advanced Laser Light Sources" and selected as societally relevant topics "Technology and Engineering", "Materials for Information Technology", "Energy" and "Health". A Program Advisory Committee nominated and selected experts as invited speakers. A session for each topic consisted of a keynote presentation, where major challenges for each field were defined, followed by further presentations outlining with examples how a combination of advanced light sources is already used.



Photographs from the EUCALL workshop "Addressing Societal Challenges using Advanced Laser Light Sources" at DESY during 26-27 April 2018.



#### **Technology and Engineering**

A major issue identified by the speakers was the necessity to observe and to characterize phase-changes that occur in materials, over multiple time and length scales. In the particular case of strain-induced phase transitions which can lead to mechanical failure, it was demonstrated that observation of the timescales at which the phase changes occur can reveal the responsible physical mechanisms – for example if the phase change within a surface takes place on a femtosecond timescale, this indicates that the phase change is driven by photoemission.

This suggests that a deeper understanding of phase changes in engineering materials could be obtained by performing joint and complementary experiment campaigns at synchrotrons, FELs and high-harmonic generation (HHG) laser-based sources. These sources have complementary specifications in terms of pulse duration, peak intensities and pulse repetition rate, and by combining them one might enable studies of mechanisms that take place over time scales from nanoseconds to attoseconds. An overview of physical phenomena and the timescales at which they take place is given on Table 1.

In addition to these requirements, the understanding of the behaviours of materials on different length scales is also of crucial importance. H. Poulsen discussed ferroelectric systems in which structures on length scales ranging from  $10^{-2} - 10^{-3}$  m (the device itself) to  $10^{-4} - 10^{-6}$  m (grain structure) to  $10^{-5} - 10^{-8}$  m (domain structure) influence electrical properties and device performance.

Figure 1 shows the application of synchrotron techniques in characterizing a 1 mm ceramic sample with different spatial and temporal resolutions. Bragg coherent diffractive imaging was presented, which allows the use of coherent x-rays to improve the possible spatial resolution in x-ray microscopy. The use of coherent methods for single particles could therefore be applied to bulk materials, if a coherent beam of high energy photons would be available. Thus there is a need for source development at x-ray FELs to deliver FEL radiation of higher photon energy, up to 100 - 200 keV, however a limitation can arise from the radiation damage that would occur, as serial crystallography is not possible with bulk grains.

Mechanism	Timescale (s)
Structural Changes	10 <sup>-6</sup> - 10 <sup>-12</sup>
Phonons	10 <sup>-12</sup> - 10 <sup>-13</sup>
Spin Dynamics	10 <sup>-13</sup> - 10 <sup>-14</sup>
Vibrations	10 <sup>-13</sup> - 10 <sup>-15</sup>
Electron Scattering	10 <sup>-13</sup> - 10 <sup>-16</sup>
Core-hole lifetimes	10 <sup>-14</sup> - 10 <sup>-17</sup>

Table 1: Physical phenomena and the timescales on which they take place.





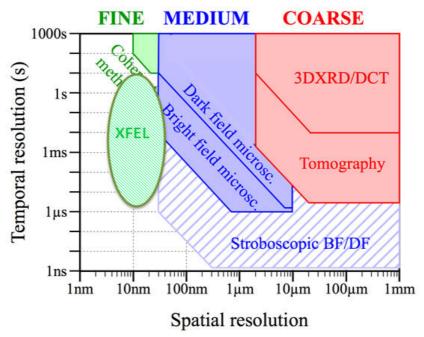


Figure 1: Performance of different x-ray techniques for a 1 mm sample at an ultimate storage ring, with a possible region where an XFEL might extend experimental capabilities (Source: H-F. Poulsen / Technical Uni. Denmark).

It was also reported that new tools are needed for modelling and simulations of the behaviour of structures from the nanometer to the micrometer scale, in order to understand how the properties of a material are influenced by its atomic structure. This type of modelling could require a large targeted collaboration, possibly as a future EU initiative.

#### **Materials for Information Technology**

Energy savings in the information technology (IT) industry due to modern energy-efficient processes are offset by increased energy consumption of new sophisticated devices. In computer memory, heating and losses are due to increased processor speeds, with a power dissipation limit of 100 W/cm², beyond which components will melt. This leads to a requirement for new concepts for non-volatile memory with fast speed and low power consumption. This provides a challenge for in-depth characterization of possible materials – static, dynamic, and in-operando. Different systems were presented, including Magnetic RAM, Phase-Change RAM, RedOx RAM and Ferroelectric RAM, and it was shown that an ensemble of complementary short and ultrashort pulse photon sources are needed to completely characterize the systems, with particular need for:

- wide range of photon energies (100 eV 10 keV)
- light polarization control
- coherence
- range of pulse lengths (ps fs)
- phase stability (down to 10 fs)





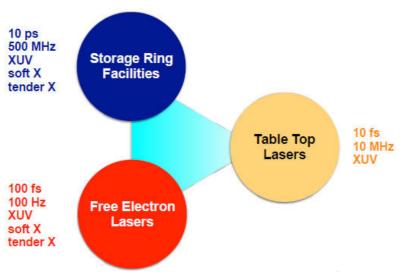


Figure 2: The characteristics of complementary light sources as required in their application to development of materials for Information Technology (Source: C.M. Schneider - FZ Jülich).

A scheme representing the synergy of light sources for these requirements is shown in Figure 2. In a particular example, the material GdFeCo was investigated for its application as magnetic RAM. Using only a single femtosecond short laser pulse, the magnetization of this material can be deterministically switched, a process, which manifest itself on the time scale of 10 - 100 ps.

While presenting the use of femtosecond x-ray pulses in investigations of ultrafast magnetism, J. Lüning emphasized that fs-slicing at synchrotron facilities is still highly in demand by users, due to the high stability of the pulses generated. Also HHG sources have particular advantages over accelerator-based sources, since the different harmonics of the laser fundamental emitted simultaneously by a HHG source cover a wide photon energy range (allowing simultaneously probing of different elements), jitter-free arrival time delay of pump and probe pulses can improve the resolution, and since these sources are easier accessible to users.

#### **Energy**

In a session dedicated to the development of new materials for solar energy conversion and photovoltaics, the fact was highlighted that the global energy consumption rate of 13.5 TW in 2001 is expected to increase to 27.6 TW in 2050 and to 43 TW in 2100. This significant increase in energy demand leads to an urgent need for carbon-neutral, sustainable energy sources. One possible future energy source is the use of materials that can perform artificial photosynthesis, meaning sunlight-induced water-splitting. The key challenge for scientists is to develop efficient and stable catalysts for this process, which implies learning how to engineer the rearrangement of chemical bonds. This often involves short-lived bond





configurations, and the processes need to be observed on multiple timescales for a complete understanding.

In the development of photovoltaic cells, laser-spectroscopy experiments were described that follow charge transitions on nanosecond to femtosecond timescales, however one limitation was pointed out in that the use of pulsed optical laser excitation to observe these charge transitions may not be directly comparable to real "operating conditions" under continuous solar excitation. It was further pointed out that studies of electronic transitions reveal some characteristics of a potential photovoltaic material, and x-ray techniques provide unique additional information by adding details of structural characteristics.

In an example of one system studied using different types of light source,  $TiO_2$  has been chosen for its potential application in photovoltaics. Time resolved x-ray absorption spectroscopy on the K-edge of Ti at a synchrotron revealed dynamics on the timescale of 100 ps, while further investigations using a fs-slicing synchrotron beamline revealed further dynamics at the 1-2 ps scale and a pre-edge feature change at 330 fs. A team in Japan repeated these measurements at the SACLA FEL and was able to resolve the time constant of the pre-edge feature to be 100 fs.

In similar measurements on the ZnO system, synchrotron x-ray absorption and x-ray emission spectroscopy reveal transient states on timescales of 200 ps to 1.2 ns, while measurements at SACLA revealed that hole-trapping takes place on timescales of 1-2 ps. Both  $TiO_2$  and ZnO have also been characterized by optical pump, UV probe measurements using HHG sources in an effort to understand charge injection mechanisms. It was emphasized that femtosecond pulsed sources in the deep UV photon energy range are required for the characterization of hole trapping in these materials.

These examples demonstrate the advantage to scientists in performing a series of measurements at complementary light sources, to resolve electronic and structural dynamics that take place over a broad range of timescales. This type of measurement campaign is essential for the development of sustainable energy sources for the future.

#### Health

In this session, the contribution of synchrotron facilities to structural biology was recognized, and the great impact that these light sources have had in solving structures of biological systems relevant to human health. The additional opportunities offered by x-ray FELs were also highlighted, including the ability to avoid radiation damage, make measurements at room temperature, use much smaller protein crystals, or even study single bio-machines without the need of crystallization. An example was shown, demonstrating that for a measurement campaign on a particular system, measurements using an FEL significantly improved the achievable spatial resolution (2.4 Å at a synchrotron; 1.7 Å at an FEL) and reduced the time needed for measurements (8 hr at a SR using 128,000 images; 0.36 hours at an FEL needing only 3500 images). Advances at FELs in Serial Crystallography have





recently been extended to synchrotron facilities, significantly improving the capabilities for structural biology also at synchrotron facilities.

Another opportunity for biological studies at advanced laser light sources is for femtosecond resolved structural dynamics, possibly to be combined with ultrafast electron measurements, to gain understanding how processes and reactions occur in space and time in these important systems. Electron spectroscopy characterisation is now being extended to the attosecond timescale using HHG optical laser sources in the XUV energy range. These measurements allow the study of complex hole formation and electronic wave migration which are observable on the attosecond to few femtosecond timescale.

A particular application was provided for medical phototherapy treatment, during which secondary electrons generated by the incident photon pulse can cause damage to surrounding DNA. Studies of electron dynamics on timescales of 2.8 – 20 fs show that following a UV pulse, this DNA damage can be mitigated by a subsequent infrared light pulse. This demonstrates the application of the sub-femtosecond light pulses in treating human disease. The speaker also emphasized the need for the development of sub-femtosecond pulses at FELs to complement this type of research.

#### **Method and Source Development**

An example of the development of FEL techniques based on optical laser experiments was given by J. van Zanthier who demonstrated that a laser-based quantum optics experiment in superradiance can be realized also at the FLASH FEL at DESY. The success of this experiment paves the way to a form of incoherent diffractive imaging at FELs, with advantages over existing techniques such as increased resolution, increased statistics and element specific imaging. An extension of the technique to using hard x-rays, which promises great potential for imaging atomic structures at FELs, has recently been tested at the LCLS FEL in the USA.

Requirements for extended capabilities of light sources were provided by several of the speakers, including:

- Maintaining beamlines with femtosecond slicing at synchrotron facilities
- HHG sources with higher photon energy (moving into the soft x-ray range)
- HHG sources with repetition rates up to several 100 kHz
- HHG sources with polarization control
- XFEL sources with photon energy range up to 100-200 keV
- XFEL sources with improved pulse-to-pulse stability
- XFEL sources with improved synchronization with external lasers
- XFEL sources with higher repetition rates (FLASH, European XFEL and LCLS-II start to address this).





#### **Summary**

The event's speakers and participants (70 in total) considered the workshop as extremely successful and provided very positive feedback. This was in large part due to substantial efforts of all of the invited speakers in preparing pedagogical presentations that suitably covered the application of different types of light source in their fields of expertise.

For all topics of discussion, clear examples were given which demonstrated the benefit of characterizing material dynamics on timescales across nanoseconds (and longer) to picosecond, femtosecond and even sub-femtosecond regimes — for which measurement campaigns across synchrotron, FEL and optical laser facilities are highly advantageous.

While a strong focus was on experiments studying multiple timescales, it is also important to characterize materials across multiple length scales, from the millimeter range to the subnanometer. The establishment of a new centre focusing on multi-scales problems for material analysis could generate tremendous synergies between different research directions and might produce new insights in this important field. Topics of such a center could involve the development of a new platform for modelling of structures from the millimeter to the nanometer scale, or the development of concepts to understand how macroscopic properties of a material are influenced by its atomic structure.

Following the workshop, it was suggested that light sources should seriously consider repeating this type of event on a regular basis, and to address a broader audience. Such a regular activity could provide novel means to inform the general public about science at light source RIs and their contribution to resolving societally relevant problems.

As a follow up activity, ELI-NP organized a further event addressing Nuclear Medicine at Advanced Laser Light Sources, which took place on 4 September 2018. Representatives from ELI-NP, Government agencies, Romanian Parliament, and medical experts attended, to discuss the challenges involved in the development and application of technologies to nuclear medicine. As an outcome, a working group was formed to deliver the designs to launch a Nuclear Medicine Center in Romania, and to include training for doctors and physicists in new nuclear techniques, nuclear safety and other topics from the field.



# Addressing Societal Challenges using Advanced Laser Light Sources 26 - 27 April 2018

Venue: Deutsches Elektronen-Synchrotron (DESY)
CSSB Auditorium, Notkesstraße 85, 22607 Hamburg, Germany

#### Thursday 26 April 2018

Time	Program	
12:00	Registration and light lunch	
13:00	Welcome to DESY – R. Brinkmann / DESY	
13:10	Introduction to the workshop – T. Tschentscher / European XFEL	
	Technology and Engineering	
13:20	3D movies on multiple length scales: a new paradigm for bulk materials – H-F. Poulsen / Technical Uni. Denmark	
14:00	Ultrafast phenomena at surfaces – M. Aeschlimann / Uni. Kaiserslauten	
14:30	Coffee Break	
	Materials for Information Technology	
15:00	Exploring ultimate time-scales in information technology: The role of ultrashort x-ray pulses — C.M. Schneider / FZ Jülich	
15:40	Quantum optics and quantum information processing implemented with FEL light — J. von Zanthier / Uni. Erlangen-Nuremburg	
16:10	Use of femtosecond x-ray pulses in understanding ultrafast magnetism  – J. Lüning / Université Pierre et Marie Curie	
16:50 – 18:00	Visit to PETRA III and FLASH	
18:00 – 22:00	Poster session and Dinner	



## Friday 27 April 2018

Time	Program
	Energy
09:00	Understanding how sunlight powers the world - The role of modern x-ray science – P. Wernet / HZB
09:40	Ultrafast laser spectroscopy of materials and devices for solar energy conversion – J. Durrant / Imperial College
10:10	Use of light sources for development in photovoltaics – M. Chergui / EPFLausanne
10:40	Coffee Break
	Health
11:10	Methods and light sources for ultrafast life science research – J. van Thor / Imperial College
11:10 11:50	Methods and light sources for ultrafast life science research – J. van
	Methods and light sources for ultrafast life science research – J. van Thor / Imperial College  Opportunities for drug discovery at light sources – M. Hennig
11:50	Methods and light sources for ultrafast life science research – J. van Thor / Imperial College  Opportunities for drug discovery at light sources – M. Hennig (leadXpro)  Tracking ultrafast electron dynamics in bio-relevant molecules – F.



# 3. Building a Targetry Network for High-Repetition Rate, High-Power Laser Facilities

High-power laser experiments at repetition rates of 1 – 10 Hz will soon become possible at facilities such as ELI, ESRF, and European XFEL, as well as at other advanced laser light sources. By this development scientific experiments exploiting the higher rates will require targets (or samples) in the quantity of few 1000 up to as high as few 100000 per year in order to take full benefit of the source capabilities and thereby to enable new discoveries. These numbers lead to a new requirement of target production facilities capable of producing a range of high-precision targets in large quantities. While in the USA certain support networks for targets supply exist, within Europe today no coordinated strategy to target fabrication exists. A possible solution could be to establish a consortium of European advanced laser light sources RIs, target suppliers and laboratories specialized in target design and characterization. This issue/need was addressed in a first EUCALL targetry workshop held in August 2016 at HZDR in Germany as a satellite to EUCALL's 1st Annual Meeting, in collaboration with members of WP6. Following up on that workshop a report was prepared. Information can be found at www.eucall.eu/target network.

A White Book article was also produced and the wider community of RI facilities was informed about this activity (DESY, ELI, European XFEL, ESRF, HZDR, and a number of facilities within the Laserlab-Europe network). A meeting of facility management staff was organized at Frankfurt airport in April 2017, in order to discuss and to determine the present and future needs of the various light sources and the level of support available to such an activity. As an outcome of this meeting the focus of this joint foresight topic has been moderately redefined to include other development areas that arise from high-repetition-rate, high-power laser experiments, such as:

- mitigation of debris and shrapnel resulting from laser-target interaction
- protection of electronic equipment from **electromagnetic pulses** generated during ultra-intense laser-target interactions
- issues related to the **target environment**, including interaction with the laser pulses to adjacent targets, and laser-induced radioactivity (activation) of surrounding components.





Participants of the 2nd EUCALL Target Network workshop at ELI-Beamlines during 29-30 May 2018.

To discuss these issues, a second workshop was held at ELI-Beamlines in May 2018 as a satellite to EUCALL's 3<sup>rd</sup> Annual Meeting. Participants of the first workshop in HZDR were invited, and prior to the event, a survey was sent to all registered participants, querying the current challenges faced by their facilities/groups regarding the aforementioned topics, the solutions they have already developed, and any open questions yet to be resolved. Responses were collected from 12 facilities, and these were reviewed by nominated conveyers who agreed to present the results during the meeting as invited speakers, and to lead open discussions on how to formulate possible future collaborations.

#### **Debris Mitigation and Back Reflection Protection**

The key challenge to overcome is that during/following a laser-target interaction, ejected material from the target (debris) can be deposited around the experimental chamber, forming coatings on optics and delicate equipment. It was also mentioned that debris can cause coatings on adjacent targets, so that nearby targets are no longer pristine when they are hit by subsequent laser shots. In some cases, larger emitted materials (referred to as "shrapnel") have been observed to cause mechanical damage to surrounding components.

It was reported that the use of cryogenic targets (for example solid hydrogen) does not generate problematic debris, but it is not suitable to all experiments. Particular types of debris shields have been developed for use at some of the involved facilities, but these shields often need to be replaced which typically is disruptive to the experiment, and can also be very expensive for high-repetition-rate experiments.

During the discussion a possible solution was proposed, which would employ a large area Mylar thin film to cover surrounding components during the experiment. These films can be procured in a large volume and can be quick, easy and cheap to replace several times during an experimental campaign. It was proposed that a collaboration could take place where such





films can be tested at a high-power laser facility, perhaps at the HED instrument at European XFEL via the HIBEF collaboration.

Another idea to help to deal with debris is to develop the ability to map the distribution of generated debris after one shot, to determine which parts of the experimental setup are most at risk. This could lead to the formulation of simulation tools to model the ejection and distribution of debris – which currently do not exist.

Participants also raised the option of the use of a gas jet to "blow" the debris away from sensitive equipment, or a liquid shield surrounding the target, which only allows transmission of the laser.

It was stated by RI operators that issues surrounding debris mitigation are of high importance and that they plan to provide beamtime to users for experiments to develop solutions. It is considered that at European XFEL's HED instrument/HIBEF such experiments can be performed offline, which means that experiments can be performed using the optical laser even when there is no FEL radiation being produced at the instrument for user experiments. It was also suggested that ELI could dedicate some of the "user-commissioning" time at its facilities for these kinds of experiments.

#### **Electromagnetic Pulse (EMP) Protection**

It was reported that, during laser experiments, an EMP produced by a single shot can cause nearby computers, controllers and detectors to shut down or damage them, and that modern equipment is much more susceptible to EMP interference than that of 5-10 years ago. The generation of EMPs and their interaction with equipment is very specific to the facility and equipment, and it is considered that an important initial activity would be to establish a platform for the sharing of information about experiments where EMPs caused problems. Participants of the workshop proposed that a certain number (10-20) of experimental parameters be defined to allow an accurate, standardized description of experiments for which EMPs have interfered.

This could lead to the formation of an online database to let user groups find out which problems have been identified and how these might affect their experiments. The data could further include how different RIs encounter EMP effects. User groups could nominate individuals who can enter this data into the database. Several participants at the meeting volunteered to move forward with this activity and begin to define the necessary experimental parameters.

Some experimental conditions were reported that can reduce the effects of EMPs, for example simply by increasing the distance between the source and sensitive equipment. Setting an oscilloscope 10 m away from the source can prevent any detrimental effect from EMPs, although this approach is not feasible for all sensitive devices.

Some groups attempt to replace as many metal components as possible, such as target positioning systems, with plastics or ceramics, and also reported the application of echo-





reducing surfaces (such as foams) inside experiment chambers – however this approach is limited by vacuum requirements in the experiment chamber.

RIs are suggested to allow experiments to measure EMP run parasitically during regular use of high-power lasers, and also to provide beamtime to dedicated campaigns to characterize EMPs. A useful step forward could be the formulation of a "Community Proposal" from the workshop participants to characterize EMP during commissioning at European XFEL's HED instrument.

#### **Target Environment**

Within the Target Environment area a number of key challenges have been identified critical to overcome in high-repetition-rate experiments:

- Alignment thermal gradients distort target frame alignment
- Solid Target Fratricide upcoming targets may be shocked or coated if too close
- Gas/liquid target injector nozzles erode, feedstock overheats
- Activation chamber components become radioactive under high-repetition-rate laser irradiation.

To address issues caused by heating of chamber components, cooling of particular components should be investigated, such as the target handling systems, diagnostic equipment and optic parts. It is also important to determine, in each experiment, the main mechanisms governing heat deposition — such as if heat is transferred via target debris, target emissions (such as x-rays, ions), or laser back-reflection.

To mitigate solid target fratricide, it was suggested that individual solid targets be separated by a distance of at least 3 mm, but of course dependent on laser pulse energy and target type. Possible mechanisms which cause fratricide should be identified, for example shockwaves, recast layers, plasma, stray light, and return current discharges. For this it would be required to determine the spatial distribution of laser energy deposited into the target. It was stated that the focal quality of the laser effects the fratricide distance, and a possible solution is to use a pre-target aperture to clip tails of the laser beam.

Erosion of gas/liquid target delivery nozzles can occur due to x-ray emission, and due to return currents. Experiments at the Vulcan laser (CLF, UK) have observed destruction of a nozzle in a single shot. Suggested solutions include the development of disposable or ceramic nozzles.

Nuclear activation of chamber components is very important to consider as a variety of radioactive isotopes may be formed with half-lives ranging from several seconds to a few days. It is of prime importance to assess the composition of the target materials and chamber components for potential activation. It is suggested to develop activation monitors for the chamber that are convenient, and monitor them regularly. Possible activation monitors could include scintillators coupled with photomultiplier tubes.





#### **Outcomes and further activities**

The participants of the workshop agreed that the discussed topics are all of high importance and expressed a high interest to collaborate further to address the identified challenges. It was asked if these topics may be addressed by a Joint Research Activities of Laserlab-Europe in its next phase, with some accelerator RIs such as ESRF and European XFEL as associate partners or observers. This would be a particularly welcome development from the perspective of EUCALL.

As initial steps, all presentations from the workshop were made available to the participants from the workshop website, and email lists for each topic were established for the participants who wanted to be involved - <a href="mailto:debris@eucall.eu">debris@eucall.eu</a>, <a href="mailto:emp@eucall.eu">emp@eucall.eu</a> and <a href="mailto:target-environment@eucall.eu">target-environment@eucall.eu</a> - which are intended to be used as discussion platforms for further collaboration on each theme.



# 2<sup>nd</sup> EUCALL Target Network Workshop 29 - 30 May 2018

**Venue: ELI-Beamlines** 

ELI-Beamlines Auditorium, Za Radnicí 835, 252 41 Dolní Břežany, Czech Republic

## Tuesday 29 May 2018

Time	Program
08:00-08:10	Meet in front of Occidental Praha Hotel for bus departure to ELI- Beamlines
08:15	Bus departure from Occidental Praha Hotel to ELI-Beamlines
09:00	Welcome and scope of workshop – T. Cowan / HZDR
09:15	Status and Targetry Needs of ELI, and ELITA Target Lab – D. Margarone / ELI-Beamlines; M. Cernaianu / ELI-NP
09:30	Status and Targetry Needs of ESRF – R. Torchio / ESRF
09:40	Status and Targetry Needs of European XFEL/HED – U. Zastrau / European XFEL
09:50	Targetry Suppliers Network – G. Schaumann / TU Darmstadt
10:10	Target Fabrication at General Atomics – N. Alexander / General Atomics
10:30	Coffee Break
	Debris Mitigation and Back-reflection Protection
11:00	Convener report – M. Cernaianu / ELI-NP
12:00	Open discussion
13:00	Lunch



#### **EMP Protection**

14:00	Convener report – D. Neely / UKRI STFC; A. Poye / ENS de Lyon; A. Garcia / HRDR
15:00	Open discussion
16:00	Coffee Break
16:30	Site visit to ELI-Beamlines and HILASE
18:30	Further exchange of information during dinner at Olivův pivovar restaurant, address: Za Radnicí 739, 252 41 Dolní Břežany
22:00	Bus transfer to Hotel Occidental Praha

# Wednesday 30 May 2018

Program

08:00-08:10	Meet in front of Occidental Praha Hotel for bus departure to ELI- Beamlines
08:15	Bus departure from Occidental Praha Hotel to ELI-Beamlines
	Target Environment (including fratricide, diagnostics)
09:00	Convener report – N. Alexander / General Atomics; R. Stephens / University of Pennsylvania
10:00	Open discussion
11:00	Coffee Break
11:30	Final discussion, future outlook
12:20	Conclusions and wrap up

12:30

13:00

**Start of EUCALL Annual Meeting 2018** 

End of Meeting, and Bus transfer to Airport



# 4. Theory and Simulation of Photon-Matter Interaction

Experiments at modern laser light sources provide new capabilities and insights, requiring significant support and advances in theory and modelling for the interpretation of results. Modern FEL instrumentation allows measurements on single particles, molecules and clusters, and also allows experiments in non-linear regimes which were not previously possible. Understanding of structural dynamics is already being pushed with femtosecond and attosecond resolved measurements becoming routine. High-power/high-energy optical lasers are being installed at synchrotron and FEL facilities, which will allow x-ray analysis of dynamically compressed materials at extreme temperatures and pressures previously not attainable at light sources. High power laser installations such as at ELI will lead to novel plasma-based sources of UV and x-ray radiation, as well as capabilities for nuclear photonics experiments.

In order to define the most pressing challenges posed to theoretical research and numerical simulations of matter in extreme fields of optical lasers, FELs, and 3rd and 4th generation synchrotron sources, EUCALL organized a workshop entitled "Theory and Simulation of Photon-Matter Interaction". The meeting consisted of invited experts presenting lectures on their perspectives on the challenges, as well as contributed talks from meeting participants. The meeting provided a very useful platform for international scientists to exchange information about their "favourite" simulation tools and demonstrating capabilities and examples, and to discuss how the tools could be developed to meet upcoming challenges.



Participants of the workshop Theory and Simulation of Photon-Matter Interaction at ELI-ALPS during 01-05 July 2018.





#### **Atoms, Molecules, and Clusters**

Characterization of single particles, molecules and clusters is now becoming possible due to the unprecedented photon flux and spatial coherence of FEL sources. High x-ray brilliance is needed to be able to measure and interpret the still very weak signal one expects from single particles, while many shots or frames of data are required for successful interpretation of that data. The planned experimental capabilities of European XFEL in particular are expected to allow experiments beyond those currently possible at existing FEL sources, for example by investigating the dynamics of such systems in the pump-probe mode with many different delay times or exploring the breadth of conformations present in a single molecule.

The light induced dynamics of atomic systems ranging from individual atoms via simple molecules (for example H<sub>2</sub>O) to complex systems like macromolecules (e.g. proteins, viruses) and clusters consisting of 10<sup>5</sup> to 10<sup>6</sup> atoms is in principle accessible to ab initio treatments such as time-dependent perturbation theory based on Hartree-Fock-Slater (HFS) orbitals, time-dependent density functional theory (TDDFT), or hybrid approaches combining (quantum) molecular dynamics and particle-in-cell simulations (MIC-PIC). Already for individual atoms, the computational demands can become challenging: The configuration space of a Xe atom consists of ~20 million multiple-hole states, leading to ~2 billion possible photon induced transitions. Further complexity arises when many-atom systems are considered. An ab initio treatment including the quantum description of chemical bonding and charge transfer between atoms in the molecule, which has been shown to be an important effect that explains the occurrence of high charge states, has so far only been demonstrated for small molecules such as CH<sub>3</sub>I [Rudenko et al. 2017] or water [Schäfer et al. 2018]. Larger systems, like macromolecules or clusters are currently treated in the individual atoms approximation (IAA) using for example the combination of the HFS solver XATOM [Son et al. 2011] with molecular dynamics code XMDYN [Jurek et al. 2016]. Approaches to go beyond the IAA and to include molecular effects are ongoing in the Theory Department at CFEL, DESY in Hamburg. Also, the extension towards extended systems with periodic boundary conditions is an active area of development.

Examples were presented of multicolour experiments where clusters are first stimulated with an ultrashort XUV pulse and then heated by a following IR pulse which causes expansion and explosion. Simulations of 3D models of these clusters are produced showing the ionization during the first few femtoseconds and resulting expansion up to 800 fs after the IR pulse.

Capabilities were also demonstrated in modelling single-shot coherent diffractive imaging, dynamic x-ray imaging and quantum imaging, non-linear atomic ionization processes and the properties of ions in exotic electron configurations (for example S<sup>8+</sup>).

Future developments for theory and simulation of finite systems in intense fields could include:





#### **Atoms**

- Electronic correlations beyond HFS
- Numerically efficient treatments of complex ionization dynamics
- Inclusions of more transitions (such as electron impact ionization in exotic ions)
- Nonlinearities, interference of transitions
- Model potentials for High- Harmonics Generation sources

#### **Molecules**

- Ab initio treatment of charge transfer and ionization dynamics in complex molecules (well defined but numerically expensive)
- Density-Functional Theory (DFT) simulations of luminescence in perovskites

#### Clusters

- Time-dependent Schrodinger Equation is not practical, so time-dependent DFT and quantum molecular dynamics should be developed
- Development of PIC codes for finite systems:
  - o atomic physics
  - o collisions, correlations
  - o quantum dynamics (currently applicable only for very simple cases)

#### **Warm Dense Matter**

Warm dense matter (WDM) can be defined as the state that is too dense to be described by weakly coupled plasma physics and yet too hot to be described by condensed matter physics. It is expected to exist within the cores of giant planets, brown dwarfs, and small stars, but is created during the solid to plasma phase transition driven by laser pulses. New laser installations at advanced light sources will therefore allow the creation of WDM and its probing with beams of x-rays.

One session focussing on research into WDM defined the planetary systems that fit into this category (giant planets such as Jupiter, Saturn, Uranus, Neptune and many extra-solar planets) and outlined the current understanding of their interiors, for example the different layers expected in each and the pressures and temperatures in each layer. Of particular interest is the unknown phase transition between molecular and liquid hydrogen, and the existence of solid metallic hydrogen in Jupiter-like planets, as well as the need for accurate equation of state data for C-N-O-H-He mixtures in ice giants like Neptune and Uranus. Full descriptions were provided about the types of x-ray experiments currently performed at synchrotrons and FELs using static and dynamic compression, as well as the theoretical models currently used to describe the experiments and the related simulations using Density-Functional Theory Molecular Dynamics (DFT-MD). Advances for theory and modelling for Warm Dense Matter should address:

 Non-perturbative, time-dependent treatment including quantum effects and correlations





- (TD)-DFT development:
  - o Temperature dependent exchange-correlation functionals
  - o Excited states
- Beyond TD-DFT methods: The Nonequilibrium Green's Function (NEGF) method is actively developed. The main challenge is to find good approximations for the selfenergy term and to make the self-energy approximations transferrable for various systems. The NEGF formalism included electron-electron correlations and the photon-matter interaction in a systematic way, which is not possible in DFT based approaches.
- Effective Hamiltonians
  - Tight binding models, Hubbard model: The numerical efficiency of these intuitive models with only few parameters comes at the price of limited transferability. Parametrizations must be benchmarked against *ab initio* calculations.
- Direct Models
  - Born-Mermin approximation (BMA), including local field corrections (BMA+LFC) need benchmarking against ab initio.
- Development of fully *ab initio* model to accurately describe WDM formation after solid's irradiation with x-rays. Simulation challenges are:
  - o correct description of atomic orbitals, ionization thresholds, and impact ionization cross sections in dense plasmas.
  - Impact of K-shell holes
  - o Transition of the electronic structure from a solid state band structure via fragmentation and ionization to a plasma state. Tight-binding models break down at high densities of excited electrons (timescales higher than 20 fs).
  - Non-applicability of periodic boundary conditions in strongly focussed laser fields.

#### **High Energy Density Physics**

Many advanced laser light source RIs involved in EUCALL are currently installing TW and PW class optical laser systems, capable of dynamically compressing materials and generating plasmas which can be characterized with an x-ray beam to understand these exotic states of matter, or to generate secondary sources of radiation for user experiments.

During the EUCALL workshop, discussions focusing on the use of FEL radiation to probe the interaction of ultra-intense optical lasers with plasmas and solids, reported that understanding of complex plasma dynamics in relativistic laser-solid interaction is limited due to uncertain initial conditions and complex transport dynamics. Current x-ray analysis techniques for these systems are indirect and incomplete, although this is expected to





change with developing capabilities of modern light sources. Simulations have limited prediction capabilities.

Understanding the generation of attosecond pulses in laser-plasmas is of high importance at ELI-ALPS, to extend the capabilities of light sources to produce intense beams of attosecond pulsed light in the x-ray energy range. The use of both gas/plasma and solid targets were reported, as well as challenges in the amplification of these relatively weak pulses, addressed via simulation and modelling.

#### **Nonequilibrium Dynamics**

Complex systems in intense radiation fields pose particular challenges for modelling and simulations. On the one hand, one needs to capture the electronic and atomic processes determining the dynamics on attosecond to femtosecond timescales. On the other hand, these systems (large clusters, biomolecules, solids, surfaces) are too big to apply atomistic simulations. Collective effects and correlations back-react on the individual particle dynamics, which has to be considered in atomistic calculations of electronic states and transition probabilities. Hence, one has to deal with a multiscale problem in both time and space. Effective models have to be developed and applied and carefully benchmarked against *ab initio* simulations.

A lecture was provided by the CFEL-DESY Theory Group, which develops theoretical and computational tools to predict the behaviour of complex systems exposed to intense electromagnetic radiation. Quantum-mechanical and classical techniques are employed to study ultrafast processes that take place on time scales ranging from picoseconds to attoseconds. Research interests include the dynamics of excited many-electron systems; the motion of atoms during chemical reactions; and x-ray radiation damage in matter. The challenges for theory description include:

- evolving band structures in systems out of equilibrium
- irradiation with hard x-rays and resulting keV excited electrons
- trade-off between computational efficiency vs. accuracy when modelling irradiated complex systems with a large number of atoms in the sample
- lack of microscopic description

A further bottleneck recognized is the lack of a universal *ab initio* description of transient electronic structures in response to nuclear dynamics. To address this, the Density Functional based Tight Binding (DFTB+) method is being applied. The description of the multiscale (spatial and temporal) physics of strongly driven complex systems was mentioned as a central challenge to theory, for example to model post-mortem relaxation processes on ps timescales, long compared to the fs excitation. The XTANT code developed at CFEL exemplifies how to combine various models and methods to address such problems.





A second session on nonequilibrium dynamics focused on the Nonequilibrium Green's Functions (NEGF) method which provides a systematic way to describe correlated systems far from equilibrium. It is also straightforward to include the radiation field. The accuracy of NEGF calculations depends on the choice of the self-energy functional for which a diagram technique is developed. This also allows connections to relativistic field theories, see also the next section.

#### **Strong fields**

The electric and magnetic fields generated by high-intensity optical laser and FEL systems currently under installation at facilities involved in EUCALL are expected to be strong enough to cause physical effects that have not yet been demonstrated experimentally, including those critical (also known as Schwinger) fields, which can substantially alter the properties of vacuum.

An invited lecture presented the quantum electrodynamical (QED) models which predict the Schwinger fields and the implications, and it was discussed that further new effects are predicted, in particular, the electron dynamics are strongly dominated by radiation-reaction and quantum effects. Although current and near-future light sources will not reach the Schwinger limit, the speed of technological advances will put this landmark within reach within the next one or two decades. Already now, subcritical strong field QED is investigated using current technology at advanced laser light sources. This can help in clarifying the fundamental and still unsolved problem of radiation reaction and its quantum origin. Challenges for theoretical modelling of these effects have been limited as calculations are feasible only for a few "special" background electromagnetic fields:

- Constant and uniform electric/magnetic fields (relevant in astrophysics)
- Coulomb field (relevant for atomic physics)
- Plane-wave fields (relevant for laser physics)

A key outcome is that operators of advanced laser light sources can be recommended to make experimental infrastructure available for users to perform measurements in the strong field QED regime for verification of the theory under development for the last several decades.

The account for QED effects in laser-plasma simulation codes (for example PIC) is an area of active research. The calculation of QED cascades in ultra-intense laser-matter interaction is not only of fundamental interest but has direct impact for example on safety considerations. The problem of radiation-reaction (runaway solutions in semi-classical treatment of the Abraham-Lorentz equation of charges in their own field) also gets a very practical one in this context. In view of these considerations, it was concluded that ultimately, a many-body quantum field theory is needed. The development of such a theory would exploit the formal proximity of field theoretical methods and the Nonequilibrium Green's Function method for many-body systems which would become natural limiting cases of this generalized concept.





The description of photon induced processes in correlated many-body systems (such as warm dense matter and hot dense plasmas), the correlated dynamics of matter in intense fields, as well as the inherent many-body character of relativistic field theories would be put on a common ground and open new possibilities for a more systematic exploration of fundamental processes in correlated systems under intense laser irradiation.

#### **Laboratory Astrophysics**

The field of laboratory astrophysics comprises both theoretical and experimental studies of the underlying physics that produce the observed astrophysical processes. Understanding of the cosmos depends on scientific knowledge in six areas: atomic, molecular, condensed matter, plasma, nuclear and particle physics. Advances in experimental capabilities of the light sources involved in EUCALL will allow experiments which simulate the conditions expected needed to understand planetary systems and star formation, stars and stellar evolution, and the galactic neighborhood.

The final session of the EUCALL workshop addressed experimental and theoretical concepts to investigate the correlated dynamics of the ionic subsystem in warm dense matter. Of particular importance is the dynamic ion-ion structure factor which can be measured in x-ray Thomson scattering experiments. Whereas optical laser driven plasma x-ray sources ("backlighter sources"), as well as SASE-FELs (non-seeded) are not capable to resolve the ion acoustic modes, experiments at LCLS using a seeded beam and monochromators have demonstrated this capability for seeded highly monochromatic x-ray sources. The interpretation of the measured dynamic ion structure factors is ongoing and requires the development of novel methods. A group at Oxford University is very active in this direction exploiting methods such as orbital-free density functional theory, fluid dynamics, and non-orthodox quantum mechanics to overcome the computational challenges posed by the need to address both the dynamic degrees of freedom as well as the static ion correlations. Since a publication from this group is currently under preparation, we refrain from giving further details here.

#### **Development of new instrumentation**

The participants of the workshop also discussed that the next proposals for advanced laser light source schemes and beamlines should be driven by important fundamental scientific questions and to provide properties exceeding present day capabilities. In particular, FEL beams with controllable polarization are desired, while it is of interest to develop further FEL sources with MHz repetition rate and to extend the repetition rate beyond to continuous wave (CW) mode. It is important to determine the ultimate achievable intensity, and photon energy for FEL radiation. For optical laser development, it will be important to developing optical laser technologies which are approaching the Schwinger limit.





#### Summary of recommendations for future activities

Important recommendations for method development include interpolation between condensed matter and hot dense matter to describe warm dense matter states, predictive simulations for generation of attosecond pulses and high harmonics sources, development of the Nonequilibrium Green's Functions for time-dependent description of ultrafast phenomena, and to exploit the formal proximity of Nonequilibrium Green's Functions and Quantum Electrodynamics to develop a many-body Quantum Field Theory. It is also recommended to allow fundamental science to drive proposals for future light source instrumentation, for example FELs allowing polarization control, increasing the FEL repetition rate to CW mode and pushing the limits for intensity and photon energy, while development of optical lasers approaching the Schwinger limit is also of high importance.

#### **Conclusion and outlook**

The EUCALL workshop "Theory and Simulation of Photon-Matter Interaction" was a very successful networking event which brought together scientists from synchrotron, FEL, optical laser facilities, as well as users of these light sources, to present the capabilities of their simulation tools, theoretical models and to discuss the current limitations and key challenges. The participants expressed interest in future meetings of this type, and also in developing new collaborations together to begin to address these challenges, in particular within clustering activities between light source RIs and university research groups.

It was suggested to organize a follow-up meeting to a larger scientific conference, and the annual DESY/European XFEL Users Meeting could be a possible host for this. Many of the EUCALL workshops participants would be able to attend such a meeting using their own travel funds. A further suggestion for a follow up meeting is to include hands on practice of theoretical simulation using various tools. Alternatively, the Helmholtz Graduate School for Hadron and Ion Research (HGS-HIRe) may be able to provide funding for a small workshop.



# Theory and Simulation of Photon-Matter Interaction 01 - 05 July 2018

Venue: ELI-ALPS

ELI-ALPS Auditorium, Budapesti út 5, 6728 Szeged, Hungary

## **Sunday 01 July 2018**

Time	Program
18:00 – 20:00	Welcome Reception at Art Hotel Szeged – (Somogyi u. 16, Szeged)

## **Monday 02 July 2018**

Time	Program
07:45	Bus departure from Novotel Hotel to ELI-ALPS
08:30	Welcome and scope of workshop – C. Fortmann-Grote / European XFEL
08:40	Introduction to ELI-ALPS, and in-house simulation efforts on Photon-matter interaction – M. Upadhyay-Kahaly / ELI-ALPS
	Atoms, Molecules, and Clusters
09:00	Controlling and imaging ultrafast electron dynamics in clusters – T. Fennel / University of Rostock
10:30	Coffee Break
11:00	Local structure analysis and luminescent study of SrZnO₂ nanoparticles - Manju / Punjabi University, Patiala
11:30	Ab initio calculation of electron impact ionization cross sections for ions in exotic electron configurations – J. Bekx / CFEL-DESY
12:00	Simulations of intense hard x-ray induced dynamics in matter – Z. Jurek / CFEL-DESY
12:30	Elliptical dichroism in non-linear atomic ionization – J. Hofbrucker / Helmholtz Institute Jena
13:00	Lunch Break





#### **Warm Dense Matter**

14:30	X-ray diagnostics of warm dense matter – R. Redmer / University of Rostock
16:00	Coffee Break
16:30	Compact High-Brightness X-ray sources for ultrafast probing of explosively driven solid-density materials by Travelling-Wave Thomson-Scattering – K. Steiniger / HZDR
17:00	X-ray Thomson scattering in non-equilibrium – J. Vorberger / HZDR
17:30	PIC Simulation of laser and Ta-Al multilayer interaction – M. Banjafar / European XFEL
17:50	Advances at EUCALL RIs – G. Appleby / European XFEL
18:10	End of session
18:45	Bus departure from ELI-ALPS to Novotel Hotel



## Tuesday 03 July 2018

Time	Program
08:15	Bus departure from Novotel Hotel to ELI-ALPS
	Nonequilibrium Dynamics I
09:00	Ultrafast transformations in matter induced by intense X-ray radiation — B. Ziaja-Motyka / CFEL-DESY
10:30	Coffee Break
11:00	Ultrafast fragmentation of $N_2^{2+}$ – M. Krishna / CFEL-DESY
11:30	X-ray-induced Thermal And Nonthermal Transitions modelled with a hybrid approach – Z. Li / MPISD
12:00	Analysis of interferometry data – T. Vinci / LULI
12:30	Rietveld Analysis of Zinc Aluminate – M. Jain / Punjabi University
13:00	Lunch Break

# Nonequilibrium Dynamics II

14:30	Towards a simulation of ultrafast electron dynamics in correlated systems – M. Bonitz / Kiel University
16:00	Coffee Break
16:30	Study of Ag doped GeSbTe thin films using X-ray photoelectron spectroscopy. – P. Singh / Punjabi University
17:00	Perovskite oxides, spin dynamics – J. Jiwuer / ELI-ALPS
17:30	Superior Photo-thermionic electron Emission from Illuminated Phosphorene Surface — S. Madas / ELI-ALPS
17:50	SIMEX – C. Fortmann-Grote / European XFEL
18:10	End of session
18:45	Bus departure from ELI-ALPS to Novotel Hotel



## Wednesday 04 July 2018

Time	Program
08:15	Bus departure from Novotel Hotel to ELI-ALPS
	High Energy Density Matter
09:00	Attosecond pulse generation and amplification in laser plasmas — A. Andreev / ELI-ALPS
10:30	Coffee Break
11:00	Nanometer probing of ultrahigh intensity ultrashort pulse laser interaction with solid density plasmas, by SAXS using XFELs – T. Kluge / HZDR
11:30	Investigating the influence of the picosecond leading pulse edge on ultra-intense laser heating of solids – M. Garten / HZDR
12:00	Quasi-phase matching of high-order harmonics using multiple gas jets under loose focusing conditions – M. Dumergue / ELI-ALPS
12:30	Elliptically polarized high-order harmonics generated in aligned CO₂ molecules − A. Nayak / ELI-ALPS
13:00	Lunch Break
14:30	Tour of ELI-ALPS facility
16:30	Bus departure from ELI-ALPS to Novotel Hotel
17:00	Free time
19:00	Further discussion during workshop dinner at "Roosevelt téri Halászcsárda" Restaurant  Address: Roosevelt tér 14, 6720, Szeged
	www.sotarto-halaszcsarda.hu



# Thursday 05 July 2018

Time	Program
08:15	Bus departure from Novotel Hotel to ELI-ALPS
	Strong fields
09:00	Strong-Field Classical and Quantum Electrodynamics in Intense Laser Fields – A. Di Piazza / Max Planck Institute for Nuclear Physics
10:30	Coffee Break
11:00	Improved one dimensional model potentials for strong field simulations - A. Czirjak / University of Szeged
11:30	The application of worldline instantons technics for pair production from vacuum – C. Lan / ELI-ALPS
12:00	Strong Field Trident Pair Production – U. Hernandez Acosta / HZDR
12:30	Quantum description of relativistic charged particles interacting with a strong laser field in a plasma – S. Varro / ELI-ALPS
13:00	Lunch Break
	Laboratory Astrophysics
14:30	The Dynamic Ion-Ion Structure Factor of Warm Dense Matter – G. Gregori / University of Oxford
16:00	Coffee Break
16:30	Colliding laser-produced plasma (CLPP) as targets for laser-generated extreme ultraviolet sources – H. al-Juboori / Uni. College Dublin
16:50	Pair creation on a nucleus in plasma induced by a strong laser field – P. Mati / ELI-ALPS
17:10	Workshop summary and closing remarks – C. Fortmann-Grote/ European XFEL
17:40	End of Workshop
18:45	Bus departure from ELI-ALPS to Novotel Hotel



# 5. Future Strategies for Research Infrastructure Operation

Being one of the first projects addressing the overlap between accelerator- and optical laser-driven RIs, EUCALL has sparked a lot of interest and response from the corresponding communities. EUCALL supports the exchange of, and thereby enhances, operational expertise of the involved light sources, and analyses opportunities for future synergies and common activities. Beyond key ESFRI facilities, these cluster activities involve major national laser, FEL and synchrotron facilities through their direct participation and the involvement of the networks Laserlab-Europe and FELs of Europe.

In the four technical EUCALL activities – Simulation of Experiments from source to detector, Ultrafast Data Acquisition, High-Repetition-Rate Sample Delivery, and Pulse Characterisation and Control – teams from laser- and accelerator-based light sources worked successfully together to solve problems impacting the operation and use of the Advanced Laser Light Source facilities.

To disseminate the results of EUCALL to RI operators and to policy makers, EUCALL organized the Joint Foresight Workshop on "Future Strategies for Research Infrastructure Operation - The benefits of cross-community clusters: EUCALL's perspective" which focussed on the presentation of the results of the synergy analysis performed within EUCALL and discussed the future opportunities for cross-community clusters of major European research infrastructures.

#### Benefits of clustering on technical developments

The EUCALL technological WPs demonstrated that there are indeed a number of engineering and physics problems shared by advanced laser light sources that are best addressed at a cross-community level through clustering initiatives. This model is clearly relevant in a number of areas and such an approach should be systematically considered and financially supported wherever possible as it is more effective in terms of use of resources and has greater overall impact.

#### In particular:

- The SIMEX simulation tools help scientists better prepare for experiments and understand their possible outcomes ahead of time.
- UFDAC algorithms and a flexible software framework help scientists benefit from high-repetition rate experiments better by expediting the data flow from detector to storage and allowing scientists to see immediate online results, meaning they can better react to measurements as they take place.





- Automated, standardized equipment developed through HIREP gives scientists the ability to refresh samples at a 10 Hz rate and enable reliable and precise alignment of those samples with the beam.
- PUCCA diagnostic devices help users characterize their beams to enable measurements to take place at higher time resolutions and with better understanding of how they come to their results.

#### Effects of landscape analysis and standardization of instrumentation data

WP3's landscape analysis of the advanced light sources in Europe showed the complementarity of accelerator-based and optical laser-based facilities. The consolidated promotion of the sources and research opportunities to user communities, as exemplified by the inclusion of Laserlab-Europe and ELI's beamlines and instrumentation into the Wayforlight database, should be promoted and pursued on a long-term basis. The synergies in terms of research potential and the missing capabilities identified by the experts consulted by EUCALL should be further explored and promoted. Finally, the initial landscape analysis performed within EUCALL should be reviewed and updated periodically with the support of expert users.

Particular recommendations following analysis of WP3's landscaping spreadsheet:

- Keep broad range of instruments to enable and support broad scope of scientific applications. Multiplicity of certain instruments is a benefit, for example in order to respond to very high demands
- Request for local and international, but also highly specific and multi-purpose facilities, to respond best to community needs
- Encourage experimental campaigns making use of different type of light sources for complementary measurements (for example as fs ps ns time scales)
- Develop FELs/laser instruments such as to reach the stability, operational performance and versatility of synchrotron instruments
- Standardize instruments through joint developments and sharing of know-how to enable easier access and more effective use. Enable to use complementary facilities using known techniques.
- Consider using compact (laboratory based; possibly local RI) sources for precharacterization before performing experiments at large-scale, often highly oversubscribed RIs.

#### RI clusters and innovation

EUCALL confirmed the significant role advanced light sources can play in the innovation process through technological development, the provision of access to industrial companies and promotion of the exploitation of their results for market-oriented applications. Advanced light sources face essentially the same challenges in the development of their





innovation potential. Approaching them at a cross-community level through sustained networking activities will help develop and disseminate best practices and should therefore be promoted. The conditions for the combined use of the facilities or for joint promotion and exploitation of results should be further explored and supported wherever it is expected to create greater impact on innovation.

Recommendations to increase the innovation potential of ALL-RIs:

- Disseminate 'Best practices' to new/starting RIs. The most important are:
  - o Carefully evaluate all technical, scientific and software developments with respect to their potential technology transfer to industry
  - Train researchers about which inventions should be protected and which are more suitable for direct publication
  - o Avoid generation of too many expensive patents which are later abandoned.
  - Dedicate staff to support, perform, analyse and report proprietary research for commercial users. If this is not possible, provide clear and attractive incentives for RI staff to perform this work
  - Engage with external mediator companies where possible/applicable, interfacing third part customers and RIs to reduce burden on staff.
- Establish a networking of RI technology transfer offices to initiate new types of collaborations, such as:
  - Develop and introduce new and common key performance indicators to measure economic impact of RIs
  - Develop/recognize elements for technology transfer (TT) policies to be adhered to by different RIs or even be used for a common TT charter
  - Establish a platform to discuss/disseminate innovations/patents/spin-offs of RIs within EU-wide network of RI TT offices
  - o Gather former light-source scientists now working in industry (knowledge transfer to industry) for better engagement of potential commercial users.
- Develop and disseminate training programs for young researchers with the aim to sensitize them for identification of relevant intellectual property, ways of protection and commercialization

Following the meeting in Brussels, the beneficiaries and associate partners of EUCALL signed a Letter of Intent to continue their collaboration under the "EUCALL Forum". A Memorandum of Understanding describing the underlying principles of the EUCALL Forum is under development and is foreseen to be signed in November 2018.





# Future Strategies for Research Infrastructure Operation

The benefits of cross-community clusters: EUCALL's perspective

#### 06 September 2018

**Venue: Renaissance Brussels Hotel**Rue du Parnasse 19, 1050 Brussels, Belgium

Time	Program
12:00	Registration, coffee and light lunch Exhibition and discussion of EUCALL technical results
12:50	Welcome – T. Tschentscher / European XFEL
13:00	Expectations from RI clusters – P. Froissard / European Commission
13:10	A brilliant future for Europe: Advanced laser light sources – T. Tschentscher / European XFEL
13:30	Exploring ultimate time-scales in information technology: The role of ultrashort x-ray pulses – C.M. Schneider / FZ Jülich
13:45	Panel discussion  Value added through cross-community activities – Highlights of EUCALL  - Wayforlight database – C. Blasetti / Elettra  - Landscape analysis – M. Gühr / Uni. Potsdam  - Technical results & experience exchange – S. Pascarelli / ESRF  - Innovation at RIs – A. Bonucci / European XFEL and A. Hála / ELI
14:30	Coffee Break Exhibition and discussion of EUCALL technical results
15:00	Worldwide context – R. Falcone / American Physical Society
15:20	<ul> <li>Panel discussion (Moderation: C. Miron / CEA):         <ul> <li>Benefits of clustering on technical developments – M. Svandrlik / FELs of Europe</li> <li>Landscaping and standardization of instrumentation data – CG. Wahlström / Laserlab-Europe</li> <li>RI clusters and innovation – J. Hrušák / ESFRI</li> </ul> </li> </ul>
16:00	Summary & outlook – T. Tschentscher / European XFEL
16:10	End of Meeting

#### Future Strategies for Research Infrastructure Operation The benefits of cross-community clusters: EUCALL's perspective

#### 06 September 2018, Brussels



Contributor

**Phillipe Froissard** 



Thomas
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Claus Michael Schneider FZ Jülich



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Markus Gühr
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Sakura Pascarelli



#### Profile

Philippe Froissard is the Deputy Head of Research Infrastructures Unit, which supports the development, implementation and integration of Research Infrastructures of pan-European interest. He graduated in nuclear engineering in Grenoble (France) in 1988 and completed his PhD in nuclear physics in 1992. He worked on nuclear fusion research and particularly on radio frequency heating first at the JET Joint Undertaking in Oxfordshire (UK) and then at the Commissariat à l'Energie Atomique (CEA) in Cadarache until 1999. He joined the Directorate-General for Research in 2000 and has held since several positions in the Human Potential and International Cooperation Programmes.

Thomas Tschentscher is Scientific Director at the European X-Ray Free Electron Laser Facility in Schenefeld, Germany, and is the Director of the EUCALL Horizon 2020 project. After receiving his Ph.D. in condensed matter physics at the University of Hamburg / DESY he joined the ESRF, where he performed research in condensed matter electronic properties and hard materials properties. As a senior scientific staff member of DESY, he was a member of the European XFEL Project Team, where he is now Scientific Director since 2010 and is responsible for scientific applications, X-ray optics, and optical lasers. Since 2011, he supports the implementation of large-scale physics research infrastructures in the European science area. He chaired the Steering Committee of the FP7 project CRISP, currently serves on the Scientific Advisory Committees of the LCLS and the ELI-Beamlines facilities, the EuPRAXIA Horizon 2020 project, and as a member of the ELI International Scientific and Technical Advisory Committee.

Prof. Dr. Claus M. Schneider is director at the Peter-Grünberg Institute at the Research Center Jülich. He received his Ph.D. in Physics from the Free University Berlin in 1990. After a postdoctoral period at Simon Fraser University in Vancouver, he became group leader at the Max Planck Institute Halle/Saale and obtained his habilitation in 1996. He moved on to the Leibnitz Institute of Solid State Research in Dresden as a head of the Department "Thin Films and Nanostructures", before taking on his current position in 2003. He is full professor at the University Duisburg-Essen within the University Alliance Ruhr (UAR) and adjunct professor at the University of California in Davis. His field of expertise concerns the electronic and quantum properties of materials for applications in information technology with an emphasis on spin-related phenomena and a methodological focus on photon-based techniques involving synchrotron and laser radiation.

Cecilia Blasetti is International Project Officer at Elettra, and she also assists scientists from Elettra and FERMI light sources in preparing their applications and contributes to strategic reporting for national and international funding agencies. After a master in Solid State Physics and a Ph.D. in Nanotechnology, she moved to the Grants Office as assistant project manager of the FP6 and FP7 Integrating Initiatives coordinated by Elettra (IA-SFS, ELISA and CALIPSO projects). She coordinated the <a href="wayforlight.eu">wayforlight.eu</a> portal from the beginning and she now follows its developments in the Horizon2020 CALIPSOplus and EUCALL projects, as well as within the LEAPS initiative, in which she leads working group n.5 "User services and impact assessment".

Markus Gühr is Lichtenberg Professor for Experimental Quantum Physics at Potsdam University, financed by the Volkswagen foundation. He received his Ph.D. in Physics from Freie Universität Berlin in 2005 and worked as postdoctoral researcher at Freie Universität Berlin and Stanford University. In 2007, he became Staff Scientist at SLAC National Accelerator Laboratory. In 2011, he received an Early Career Award from the US Department of Energy, Office of Science. In 2015, he joined the faculty at Potsdam and serves as a consulting Professor in the Photon Science Faculty at Stanford University. He is a member of the LCLS science advisory board and proposal review panel.

Sakura Pascarelli is Head of the Matter at Extremes Group within the Experiment Division of the ESRF and also scientist in charge of the X-ray absorption spectroscopy beamlines BM23 and ID24. She received a Laurea in Physics at the University La Sapienza (Rome, Italy) and a Ph.D. degree in Physics at the University Joseph Fourier (Grenoble, France). Her research today deals with studies on matter at extreme conditions of pressure, temperature, and magnetic fields using principally X-ray Absorption Spectroscopy and X-ray Magnetic Linear and Circular Dichroism.





Aleš Hála ELI-Beamlines



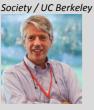
Antonio Bonucci
European XFEL



Roger Falcone

American Physical

Society ( U.G. Barkelov



Michele Svandrlik

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Claes-Göran Wahlström

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Aleš Hála has been working for ELI Beamlines as a head of the technology transfer unit since 2012. His main responsibilities include commercialisation of research projects with business potential and communication with industrial companies. Before joining the ELI Beamlines project, Aleš launched the CzechAccelerator project to support local start-up companies wishing to gain business experience in the USA and Asia. He gained international experience in Brussels, where he spent four years as a director of the regional office of CzechInvest agency in Benelux.

Antonio Bonocci is responsible for the Industrial Liaison Office of the European XFEL since 2017. After graduating in Aerospace Engineering at the University of Pisa, Antonio Bonucci joined SAES Getters in 2000, and was responsible for the modelling and simulation department. From January 2008, he was responsible for Application Engineering and System Analysis (AESA). In 2013, he began working in technology and opportunity scouting. During this work experience, he dealt with products that are used in applications addressing different scientific and technological content. In 2014, he joined European XFEL as In-Kind Contributions Supply Chain Manager.

Roger Falcone is a Professor of Physics at the University of California, Berkeley, and an affiliated faculty member of Berkeley's Energy and Resources Group and Applied Science and Technology Program. He chaired the Physics Department from 1995-2000. As of January 2018, he is a Professor of the Graduate School at Berkeley. He received his A.B. in Physics (1974) from Princeton, and Ph.D. in Electrical Engineering (1979) from Stanford and was a Marvin Chodorow Fellow in Applied Physics (1980–83) at Stanford. Falcone is currently President of the American Physical Society (2018) and serves in the Presidential Line for APS during 2016–19. He was the Director of the Advanced Light Source X-ray synchrotron facility at Lawrence Berkeley National Lab from 2006–2017. He was elected to the American Academy of Arts and Sciences and is a fellow of the American Physical Society, Optical Society of America, and the American Association for the Advancement of Science.

Michele Svandrlik is presently the Director of the FERMI Free-Electron Laser at Elettra, Trieste, Italy. After his degree in electronic engineering he joined the radiofrequency group at Elettra, where he was responsible for the design of the Elettra RF cavities, first for the normal conducting main RF system and then for the superconducting third harmonic system. Then he was project leader for the Elettra new full energy injector, a 2.5 GeV booster synchrotron, delivered in 2007 on time and on budget. He was later appointed as Head of Engineering of the FERMI FEL project and since 2011 he serves as Director of the facility. Since 2012 he is member of the FELs of Europe Steering Committee, which he chairs since July 2017.

Claes-Göran Wahlström is since 2012 the coordinator of the Laserlab-Europe consortium, which brings together 33 leading organisations in laser-based inter-disciplinary research from 16 countries. He is Professor of Physics at the Lund University, where he is the head of the Atomic Physics Division, at the Department of Physics, and of the Lund Laser Centre. His own research addresses ultra-high intensity laser—matter interactions and laser-driven particle acceleration in particular. Since 2010, he is an elected member of the Royal Swedish Academy of Sciences.

Dr. Jan Hrušák is working at the Czech Academy of Sciences and since 1995 has accumulated sizable experience in the fields of research infrastructures. He holds a Ph.D. in Chemistry from the TH Merseburg (Germany) specialized in computational chemistry, and he has been deeply involved in research policies including strategy setting for the operational program "Research and Development for Innovation". Since 2007, he has been a member of the "Council for Large Research Infrastructures", an advisory body at the Ministry of Education, Youth and Sports (MEYS), the authority for research in the Czech Republic. He has served for more than ten years as the Czech delegate to European Strategy Forum on Research Infrastructures (ESFRI), the last four years also acting as an EB member. More recently he was chairing the ESFRI ad hoc Working Group on Long Term Sustainability of RIs. In June 2018, he was elected by the delegates and appointed new Chair of ESFRI, and his two-year term will start on 1 January 2019.





# 6. Conclusions, recommendations and future activities

This section summarizes the most important conclusions and recommendations for the activities addressed in this report.

# **6.1 Addressing Societal Challenges Using Advanced Laser Light Sources**

During the "Addressing Societal Challenges using Advanced Laser Light Sources" workshop at DESY, clear examples were given that demonstrated the benefit of characterizing material dynamics on timescales across nanoseconds (and longer) to picosecond, femtosecond and even sub-femtosecond regimes — for which combined measurement campaigns across synchrotron, FEL and optical laser facilities are highly advantageous. It is also important to characterize materials across multiple length scales, from the millimeter range to the subnanometer. A potential new synergy would be the establishment of a new center focusing on multi-scale problems for material analysis, which could include the development of a new platform for modelling of structures from the millimeter to the nanometer scale, and concepts to understand how macroscopic properties of a material are determined by its atomic structure. Advanced laser light sources are strongly encouraged to repeat this type of meeting on a regular basis, and to address a broader audience, as a novel approach to inform the general public about science at light source RIs and how RIs serve society's needs. A follow-up activity, focusing on Nuclear Medicine, enabled constructive exchange between operators of ELI-NP, medical experts and research scientists.

# 6.2 Building a Targetry Network for High-Repetition Rate, High-Power Laser Facilities

EUCALL's Targetry Network workshops, held as satellites to the 1st and 3rd EUCALL Annual Meetings have resulted in recommendations for immediate first activities in how a consortium of light source RIs could collaborate to address pressing challenges that arise during high-repetition-rate, high-power laser experiments. Debris mitigation could be achieved through Mylar thin films covering components; gas-jets to "blow" the debris away, or a liquid shield surrounding the target. Modelling the ejection and distribution of debris would also be beneficial. Electromagnetic pulse protection could be supported by the sharing of information and an eventual database about experiments where EMPs caused problems. RIs are suggested to measure EMPs parasitically while operating high-power lasers, and also to provide beamtime to dedicated campaigns to characterize EMPs. Problems in the target environment can be addressed by investigating the mechanisms





governing heat deposition and developing cooling techniques. Mechanisms governing solid target fratricide should be determined, and apertures to clip tails of the laser beam can be considered. The composition of the target materials and chamber components should be carefully analyzed for potential nuclear activation, while it is also recommended to develop activation monitors for the chamber. These recommendations could form Joint Research Activities for Laserlab-Europe, with ELI, ESRF, and European XFEL as associate partners. The establishment a consortium of European advanced laser light sources RIs, target suppliers and specialized laboratories is recommended as a future task to ensure the supply of targets for high repetition rate experiments.

### 6.3 Theory and Simulation of Photon-Matter Interaction

The participants expressed interest in future meetings of this type, and also in developing new collaborations together to begin to address these challenges, in particular within clustering activities between light source RIs and university research groups. It was suggested to organize a follow up meeting to a larger scientific conference, and the annual DESY/European XFEL Users Meeting could be a possible host for this. Important recommendations for method development include interpolation between condensed matter and hot dense matter to describe warm dense matter states, predictive simulations for generation of attosecond pulses and high harmonics sources, development of the Nonequilibrium Green's Functions for time-dependent description of ultrafast phenomena, and to exploit the formal proximity of Nonequilibrium Green's Functions and Quantum Electrodynamics to develop a many-body Quantum Field Theory. It is also recommended to allow addressing important fundamental scientific questions to drive proposals for future light source instrumentation.

# **6.4 Future Strategies for Research Infrastructure Operation**

EUCALL has shown that a number of physics and engineering problems shared by advanced laser light sources can be best addressed at a cross-community level through clustering initiatives, and such an approach should be systematically considered and financially supported wherever possible as it is more effective in terms of use of resources and has greater overall impact.

EUCALL's promotion of instrumentation and research opportunities to user communities, as exemplified by the inclusion of Laserlab-Europe and ELI's beamlines and instrumentation into the Wayforlight database, should be disseminated and pursued on a long-term basis. The synergies in terms of research potential and the missing capabilities identified by the expert users in Deliverable 3.2 should be further explored and promoted. It is also recommended that EUCALL's initial landscape analysis should be reviewed and updated periodically with the support of expert users.





Advanced light sources face essentially the same challenges in the development of their innovation potential, and addressing these challenges at a cross-community level through sustained networking activities will help develop and disseminate best practices and should therefore be promoted.

# 7. Summary and Outlook

The activities carried out within EUCALL WP3 have resulted in the identification and investigation of three topics of particular interest for the further development of the advanced laser light sources in view of their scientific and innovative potential. These activities revolved around a total of seven workshops addressing those three thematic areas. The workshops brought together EUCALL partners and scientists, engineers and managers from the community and other research infrastructures. Feedback received from the participants was overwhelmingly positive and several suggestions for further workshops have been collected.

The "Societal Challenges" event gave participants the opportunity to review how the various facilities and research methods, and in particular how the suite of advanced laser light sources, contribute or may contribute to addressing societal challenges. This activity highlighted future directions of research and collaboration and even concrete proposals for actions were made. Similar events with different focus and direction may be repeated in the future.

The prospect of high-repetition rates at the new advanced laser light source facilities triggered the creation of a "Target Network" as another significant activity within WP3. The full scientific exploitation of these facilities and their use by small- and medium-sized research groups will require solutions to address the challenges that come with high-repetition-rate experiments, such as debris, EMP, or simply the provision of the adequate number of samples/targets.

With the new possibilities offered by the suite of advanced laser light sources it becomes more and more relevant to put a focus on "Theory and Simulation" in order to prepare, conduct and analyze experiments at these facilities. Current theoretical methods and standard simulation tools are facing their limits and new developments and breakthroughs are needed to keep pace with experimental progress. Without advances in that area it will become difficult to efficiently prepare experiments and to properly analyze experimental data.

Overall, EUCALL has provided the demonstration that advanced laser light sources share a number of common physics and engineering problems, as well as operational challenges that can best be addressed at a cross-community level through clustering initiatives. The project and its results make a strong case for future support of cross-community initiatives by European and national funding agencies. EUCALL WP3 recommends such approaches be





systematically considered and financially supported wherever possible considering their strong added-value and impact.

The formation of the "EUCALL Forum" will ensure some continuation of EUCALL's activities and may give the impetus in specific areas for new activities such as those identified as joint foresight topics within EUCALL and presented in this report. The "EUCALL Forum" will adequately complement Laserlab-Europe and LEAPS, which span the entire advanced laser light source landscape, and certainly provide strong integrating and networking platforms for pushing many of the activities foreseen in the wake of the EUCALL project.