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Work Package 4 – SIMEX

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Design Report and Advanced Simulation Software – Short Pulses Interaction

Lead Beneficiary: European XFEL

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Abstract – We present a design for integrated simulations of an x-ray scattering experiment probing high power femtosecond laser pulses interacting with solid matter by small-angle x-ray scattering. Coherent x-ray pulses as delivered by an x-ray free-electron laser and their propagation through beamline optics are simulated with the simulation framework `simex_platform`. High power femtosecond optical laser pulses interacting with a solid density target are simulated with a particle-in-cell code. We trace x-ray photons scattering from the laser excited plasma using a MonteCarlo simulation and synthesize a scattering image. We present the involved simulation codes and their interfaces. An experiment to be simulated is outlined taking into account parameters of optical lasers and x-ray pulse properties available at the European X-Ray Free-Electron Laser.

1 Introduction

Ultra-short pulsed high power lasers (HPLs) typically deliver laser pulses in the infrared (800 nm to 1000 nm) at pulse durations below one picosecond. Today's high power lasers [1] can reach intensities of up to 10^{21} W/cm^2 on spot sizes of a few microns and pulse durations on the order of a few tens of femtoseconds.

Despite their intensity, these sources usually do not penetrate a solid density target but rather create a plasma at the target front side, accelerating electrons to relativistic energies in the strong electric field of the laser [2] and pushing them into the target via the $\vec{v} \times \vec{B}$ force once the velocity v approaches the speed of light [3, 4].

The generation of relativistic electrons at the front side, the transport of electrons through the target and the subsequent formation of a sheath of electrons at the target rear side all happen on time scales below a few hundred femtoseconds [5]. They can create plasma instabilities [6], ionize and heat the target bulk [7], generate strong magnetic fields or drive shocks inside the target.

These phenomena can potentially be studied with high spatial resolution of a few nanometers and temporal resolutions of a few femtoseconds using x-ray lasers [8, 9] such as the European X-Ray Free Electron Laser (XFEL).

The particle-in-cell (PIC) method [10] is an advanced simulation method to study the interaction of a HPL with a solid density target. Realistic 3D PIC simulations of laser-irradiated solid density

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plasmas require Petascale computing capabilities and produce hundreds of Terabytes of data [11].

Within the SIMEX workpackage of EUCALL we interface particle-in-cell (PIC) codes such as `PIConGPU` [12, 13] that describe the solid density plasma to codes that model the generation and propagation of XFEL pulses to generate synthetic scattering signals from free and, in the future, bound electrons. The interfaces, which are based on the openPMD [14] meta data format, are part of the software suite `simex_platform` [15], developed in a collaborative effort within SIMEX. A detailed description of `simex_platform` is given in the documentation available via the software repository [15] and in the technical milestone M4.1.

As a first test of the simulation capabilities of `simex_platform` free electron density data from a PIConGPU simulation of the interaction of a short-pulse laser system[1] available at the High Energy Density (HED) instrument [16] at the European XFEL will be used to compute a synthetic scattering signal in a Small-Angle X-ray Scattering (SAXS) geometry.

2 Photon-Matter interaction

2.1 Optical Laser

The short-pulse optical laser-plasma interaction is modeled with `PIConGPU` [12].

`PIConGPU` is an Open Source [13] explicit, relativistic 3D3V[2] particle-in-cell (`PIC`) code which can simulate the interaction of high power, ultra-short laser pulses with matter. The simulations will assume realistic parameters for the optical laser system at the HED instrument at European XFEL. The most important parameters are summarized in Table 1.

wavelength	800 nm
pulse duration (fwhm)	15 fs - 80 fs
focus size (fwhm)	3 μm
temporal profile	Gaussian
spatial profile	Gaussian
pulse energy	2 mJ
prepulse contrast	$\approx 10^{-4}$ (energy)
intensity	10^{17} W/cm^2

Table 1: European XFEL HED pump-probe laser parameters for optical laser-matter interaction simulations

HPL pulses are defined by their time dependent magnetic and electric field components. Their evolution is governed by the Maxwell equations [17]. A PIC code solves these partial differential equations on a regular mesh (usually Cartesian) using e.g. finite difference time domain techniques [18].

[1] see details below

[2] 3D3V denotes the 6 dimensional phase space spanned by 3 position vector components and three velocity vector components

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2.2 X-ray Laser (Scattering)

In principle, all imaging techniques employed for probing the interaction of `HPL` lasers with targets can be used in the case of ultra-short pulse lasers as well. However, some of these techniques are limited to slowly varying plasma conditions (in comparison to the ultra-short laser pulse duration) and thus are not suitable to capture fast, transient processes. Moreover, atomic processes, multiple scattering, velocity-dependent scattering and non-equilibrium plasma conditions cannot always be taken into account with existing modeling techniques, especially if the x-ray laser pulse itself interacts with the plasma.

Thus, for ultra-short laser pulses x-ray interaction will in addition to existing techniques be modeled via a Monte-Carlo photon interaction model. Each photon is described by its wave vector and a phase[3].

The x-ray pulse is described by temporally and spatially varying electric fields (amplitude, polarization, and phase). At discrete points in time, the field distribution in a plane perpendicular to the laser axis is converted into a photon distribution using a conversion tool contained in `simex_platform`. These photons are then tracked through the volume simulated by `PIConGPU` using the software `parataxis`. Table 2 gives an overview over the expected x-ray pulse parameters at the HED instrument at the European XFEL.

photon energy	6 keV - 12 keV
pulse duration	$\approx$ 10 fs
focus size (fwhm)	2 μm - 200 μm
rel. bandwidth	10^{-3} (SASE) - 10^{-5} (seeded)
photons/pulse	10^{12}

Table 2: X-ray pulse parameters for the HED instrument at the European XFEL

In describing the interaction of coherent x-rays with the laser excited plasma, we focus on scattering processes, predominantly Thomson scattering from free electrons. Further atomic processes, e.g. K-shell ionization and resonant scattering will be considered later when detailed atomic modelling using the scFLY code [19] has become part of the simulation capabilities. This is currently under development.

The scattering signal will be processed to infer information about the microscopic and macroscopic state of the plasma during and after the optical laser-plasma interaction. Photons are scattered according to predefined scattering functions that depend on the local properties of the matter irradiated by the HPL. In the most simple case, the local free electron density is used as an input for calculating the probability for Thomson scattering from free electrons.

There are several methods that already are or will in the future be implemented for scattering. We list them below in order of ascending generality (and technical difficulty). Due to time limitations only some of these methods will be implemented during the EUCALL project, but will be added to PIConGPU for future inclusion into `simex_platform` .

1. 3D Fast Fourier Transform of electron density

2. Ex-situ scattering using stand-alone Monte-Carlo photon scattering

[3] In the future, the photon model will also include polarization.

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3. In-situ scattering using a modified particle-in-cell algorithm and far field Lienard-Wiechert potential calculation
4. In-situ scattering using Monte-Carlo photon scattering
5. In-situ scattering using Monte-Carlo photon scattering with absorption and emission of photons

Ex-situ Fast Fourier Transforms have been implemented using the `LiFFT` library [20] and can be performed in a post processing step on `openPMD` outputs of the electron density. Implementation in `simex_platform` is currently under discussion.

Ex-situ scattering is performed by the `paraTAXIS` code. The code is still in closed source development and is planned to be released as open source within the EUCALL funding period. It uses the same libraries and techniques as `PIConGPU`. Specifically, it can read `openPMD` [14] files via `libSplash` [21] and traces photons through a mesh using `libPMacc` [13]. One can define an arbitrary interaction using a C++ function object. The current code version provides Thomson Scattering from free electrons based on the local electron density. Photon scattering is computed via repeated Monte-Carlo evaluation of the scattering function, allowing for multiple scattering.

In-situ scattering using Lienard-Wiechert potentials will be based on an already existing in-situ Lienard-Wiechert potential calculator plugin to `PIConGPU` [22]. This method will serve mainly as a cross check to the other methods. It involves a modification of the PIC algorithm that will be implemented in the future. The method allows to compute arbitrary angular far field scattering spectra during the interaction of the HPL with matter.

An implementation of in-situ Monte-Carlo photon scattering in `PIConGPU` would be based on the techniques developed for the `paraTAXIS` code. Here, the main issue is the large memory consumption by the photons traced while the simulation is running.

In addition to elastic scattering of photons from electrons, excitation of ions, absorption and emission of photons via bound-bound transitions, bound-free transitions (photo-ionization, Auger decay, shake-off processes, recombination), and free-free transitions (bremsstrahlung) will be considered in the future. The latter are incoherent processes contributing to the background radiation and their consideration is hence an important step towards a more realistic simulation of the scattering signal.

In summary, the outlined framework of physical models will in the future enable fully kinetic in-situ radiation transport modeling in a particle-in-cell code. As discussed, development of these capabilities is ongoing and completed tools will be made available in `simex_platform` and `PIConGPU`. Compatibility of all software packages will be ensured by reuse of existing libraries and the common meta data format `openPMD`.

3 Simulation workflow

The simulation workflow is depicted in Fig. 1. The x-ray pulse generation and propagation is modeled in `simex_platform` with the corresponding simulation codes. The simulated wavefronts are evaluated at the target surface and converted into a photon distribution. The photons are then propagated through the target. At discrete timesteps, each photon's wavevector undergoes a change in magnitude and direction with a certain probability, given by the Thomson scattering cross section [17]. In this way, multiple scattering events that become important especially in compressed regions of the target, are naturally included. Finally, the photon wavefunction is collapsed

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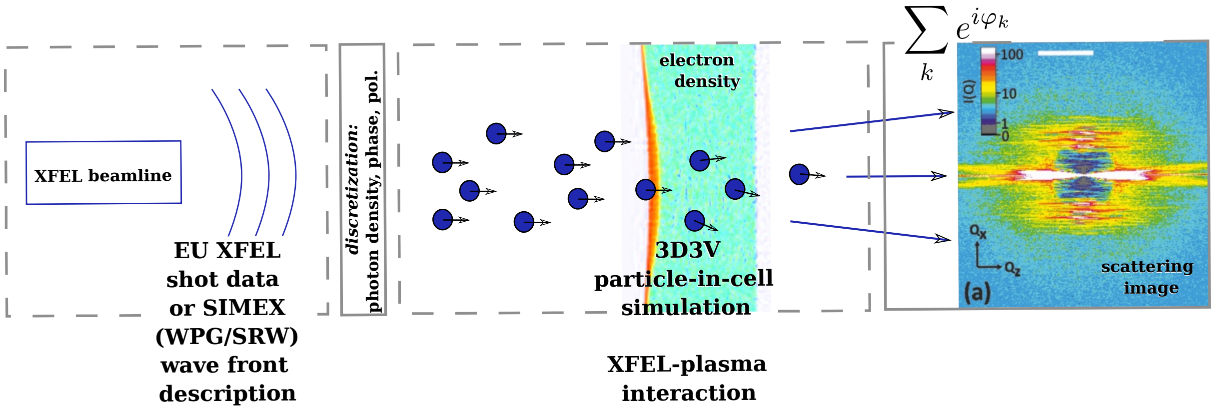

Figure 1: Block diagram for integrated simulations of x-ray scattering from a high power laser excited plasma.

onto the detector plane and integrated over the exposure time to obtain the simulated scattering image.

4 Experimental scenario

We briefly outline an experiment that we plan to simulate with the tools described above. The experiment would be carried out at the HED instrument at the European XFEL. We propose a SAXS setup, illustrated in Fig. 2, where a thin metal foil is first excited using the short pulse HED PP laser and subsequently probed by XFEL photons. The choice of the target material depends on the precise x-ray photon energy. The target material's K-shell absorption edge should be located slightly below the probe's wavelength to limit x-ray absorption. In resonant SAXS, the target material's K-shell transitions must match the x-ray photon energy. Assuming a photon energy of 8 keV, copper is a suitable target material for normal SAXS and resonant SAXS.

The HED PP laser will create a plasma of a few to ten micrometer size in the transverse dimension with respect to the XFEL beam. Hence, we choose 10 micrometer for the focal spot size to irradiate the full plasma length. A relative bandwidth of $\approx 10^{-3}$ in SASE mode, corresponding to a few eV in absolute energy is suitable for a resonant SAXS experiment to ensure efficient excitation of all involved transitions. This bandwidth is also adequate for non-resonant SAXS.

Through observation of distinct features in the scattering signal being signatures of resonant modes and instabilities in the plasma, we will extract information about these modes such as their amplitude and growth rate under varying experimental conditions such as laser power, incidence and probe angles. Fig. 3 shows three simulated scattering patterns emerging from interaction of coherent x-rays with different types of plasma instabilities [8]. It should be noted that these simulations make idealistic assumptions about the properties of the x-ray probe. An important aspect of this work is the question if the observed characteristics will remain so clearly distinct if realistic simulated pulses are employed in the scattering simulation. Comparison to experimental data will serve as a validation check of the simulation chain.

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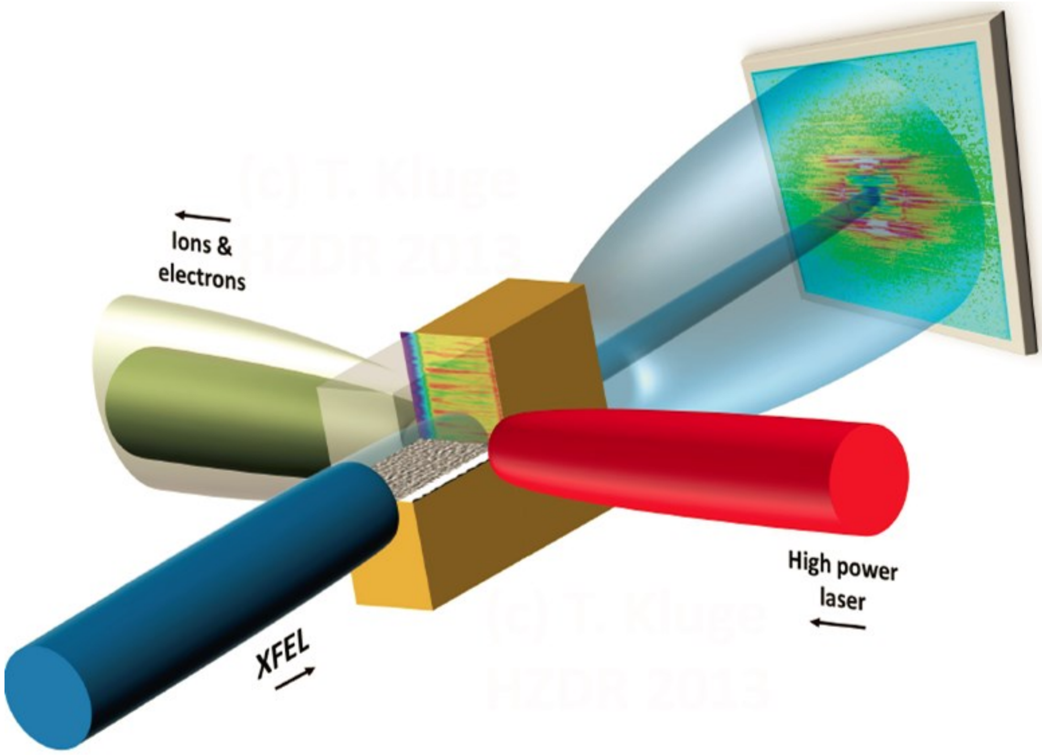

Figure 2: Schematic rendering of the proposed experiment to be simulated. Ultra-short pulsed optical laser radiation (red beam) creates a plasma layer on a metal foil's surface and accelerates electrons and ions. The XFEL beam (blue) probes the plasma perpendicular to the optical laser axis. A pixel area detector captures photons scattered in forward direction.

5 Synergy aspects

The main synergetic aspect of this work is that it allows scientists interested in short-pulse laser matter interaction to simulate their work under realistic conditions regarding the physical properties of x-ray pulses, beamline optics, and x-ray detectors. In bringing together knowledge and expertise from the high-power laser-matter interaction community, x-ray optics, and small angle x-ray scattering, we create unique opportunities for exploring the parameters at which to best perform the outlined experiment and others of similar character.

As a synergetic byproduct of the simulations outlined above, a novel application for `simex_platform` has emerged, in which we will study the concept of a laser-plasma based coherent x-ray source. The PIC simulation yields the distribution of electrons that are accelerated in the laser direction up to GeV energies due to the strong electric and magnetic fields of the HPL. This data can be fed into an FEL simulation code (e.g. `genesis` [23]) to model the process of self-amplification by stimulated emission (SASE). These simulations would enable scientists to develop precise and realistic concepts for such a laser based FEL.

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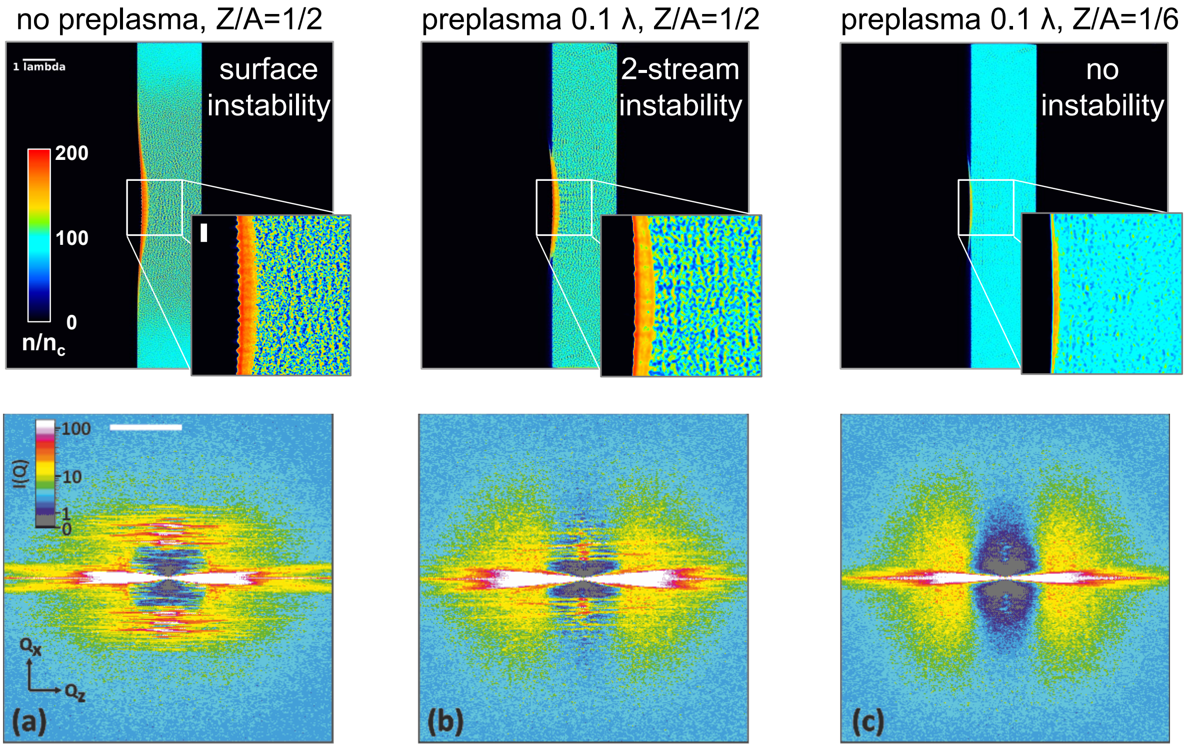

Figure 3: PIC simulations of the electron density (top) and forward scattering patterns (bottom) for various types of laser-plasma instabilities.

6 Summary and Outlook

In this report we have outlined concepts for the simulation of a SAXS x-ray scattering experiment probing the interaction of solid density matter (e.g. a metal foil) with ultra-short (femtosecond) high power optical laser radiation. The simulations describe all parts of the experiment by exploiting various codes: The generation of coherent x-ray radiation as well as the propagation from the source to the experiment through collimating and focussing optics is modelled with the corresponding codes that are already integrated in `simex_platform`. We than utilize a conversion tool that switches from a classical wavefront representation of the x-ray radiation to a photon picture, assigning each photon a wavevector and a phase. The photons are than traced through the laser generated plasma using a MonteCarlo description of scattering processes. The plasma itself is simulated with the particle-in-cell code PIConGPU. Photons escaping the target from the rear side are finally propagated to the detector plane, where a scattering image is synthesized. These simulations allow to assess the influence of realistic x-ray pulse properties on the quality of the scattering signal. We can test if the identification of plasma instabilities through characteristics of the scattering signal works under real world scenarios. The experiment we propose is designed around the expected optical and x-ray laser parameters.

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Future developments will improve the description of x-rays propagating through the plasma by including more interaction processes for absorption, scattering, and emission. It is also planned to integrate the involved simulation codes more tightly into `simex_platform`. In addition, a full detector simulation, including particle generation, charge transport and electronics will be added.

As a novel application for `simex_platform`, we plan to simulate a laser-plasma accelerator based free electron laser by feeding the output of the PIC simulation, i.e. the phase space distribution of accelerated electrons into a FEL simulation code to investigate the possibility of laser based FELs with realistic electron bunch properties.

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