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Design Report and Advanced Simulation Software – Long Pulses Interaction

Lead Beneficiary: European XFEL

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R = Report DEM = Demonstrator, pilot, prototype, plan designs DEC = Websites, patents filing, press & media actions, videos, etc. OTHER = Software, technical diagram, etc.	R
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Contents

Abstract – We present a design for integrated simulations of an x-ray absorption experiment probing dynamically compressed states of matter at tens of GPa pressure generated by high energy ($\approx 30\,\mathrm{J}$) laser pulses interacting with solid matter. We model the laser-matter interaction using 1D and 2D radiation-hydrodynamic simulations to predict the thermodynamical state of the compressed matter over the course of the x-ray pulse. These simulations are embedded in the software framework `simex_platform` to allow seamless integration into start-to-end simulations of an entire beamline experiment including x-ray pulse propagation in the beamline and detector response. The involved simulation codes are briefly presented.

1 Introduction

High-energy laser facilities are now becoming increasingly in demand at new generation x-ray light sources (X-FELs, 3rd generation synchrotron sources). The potential of long pulse ($\approx$100 ps – few ns) laser experiments are already yielding extreme conditions of matter well beyond the reach of static high-pressure techniques and combinations with x-ray techniques provide enticing experiments at new extreme states of matter.

Temporally shaped laser pulses interacting with overdense target material create a rapidly expanding plasma that can generate a shockwave in the ablating material. This shock wave can travel through the target at several km/s and compress the sample material to pressures reaching several hundred GPa. (For comparison, the Earth's core pressure is $\sim$ 330 GPa). By using a ramp temporal pulse, where the laser intensity is slowly increased, the temperatures generated remain much cooler than during rapid shock compression and the solid state of matter can be studied up to several TPa (1 TPa = 1000 GPa).

Long pulse laser systems are capable of reaching intensities of up to $\sim 10^{12}$ – 10^{15} W/cm^2 with pulse lengths of greater than a few nanoseconds. The pulse length and focal spot of the laser

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can depend heavily on the sample material and target package. Generally, focal spot sizes range between $\sim 100\ \mu$m up to 1 mm. With these specifications, the laser energies now required to reach the highest intensities are on the order of hundreds of joules. Table 1 summarizes the main optical pump laser parameters for shock compression experiments at the ESRF. A call for tender will be

Wavelength	1053 nm
Pulse duration	4 ns - 15 ns
Intensity	2×10^{13} W/cm^2
Pulse energy	30 J
Focus size (fhwm)	100 μm^2 - 300 μm^2
Temporal profile	Quasi-flat top
Spatial profile	Gaussian in x,y

Table 1: ESRF optical laser parameters for long pulse laser-matter simulations.

issued in 2016 for a new high-energy laser system to be installed at the ESRF, with increased energy (200 J) and frequency doubling crystals.

We design here simulations for a prototypical experiment combining a high-energy laser system and x-ray radiation from a 3rd generation synchrotron. The laser shock-compresses a tailored solid density target and the compressed matter is subsequently probed by x-rays. X-ray absorption spectroscopy (XAS) allows to monitor the compression and to characterize the electronic and structural states in the target. Through variation of the delay between optical laser pulse and x-ray probe pulse, time resolved data can also obtained.

2 Photon-Matter interaction

2.1 Optical laser and radiation-hydrodynamic codes

Nearly all of the physical processes of long pulse laser-matter interactions are described by partial differential equations that can be solved with careful construction of numerical simulation codes. Here, the laser-matter interactions are modelled with the 1D radiation-hydrodynamics computer code "Esther" [1] or the 2D code "MULTI2D" [2]. For the 1D hydrocodes, a moving mesh is applied in an arbitrary Lagrangian-Eulerian framework where the coordinates of the mesh contain the variables from which density can be calculated (mass of each zone is fixed). The most important variables considered in these codes are those associated with the extreme conditions generated by the high-power lasers: pressure (density), temperature and velocity. Feedback of these hydrocode outputs are crucial in the design and implementation of laser shock/ramp experiments with x-ray interactions.

It is vital to have an understanding of shock transit times so that accurate timing of the x-ray probe, with respect to the laser initialisation, can be made. The final density state reached by a shock, as calculated from the hydrocode simulation packages, can define the shock velocity.

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2.1.1 Esther

The Esther hydrocode was written by Patrick Combis and Laurent Videau of the CEA, Paris, France[1]. A license to use Esther can be obtained by requesting access (via email) from the authors (for academic use only).

As a necessary step for integration of hydrocode modelling in SIMEX, we have developed interfaces to Esther. An interactive input file generator sets up the configuration files for the hydrocode based on user provided information about the target and the laser pulse. After the simulation completed, a converter reformats the hydrocode data (pressure, density, temperature, and shock velocity as function of space and time) from the native format into an openPMD [3] conform hdf5 file. In this context it is worth mentioning that a new openPMD standard extension is currently being developed to facilitate the usage of openPMD as a standard format for rad-hydro codes.

2.1.2 MULTI2D

In the MULTI2D hydrocode [2], the hydrodynamic equations solved by the code are combined with a multigroup method for radiation transport. Multi is installed for unix with the requirement of several back engines (gcc, tcl-tk, gnuplot, pdflib-lite) with the code itself written in Fortran90. A GUI has been developed by the Laboratoire D'Utilisation des Lasers Itenses (LULI) at the Ecole Polytechnique in Paris, France.

2.1.3 Obtaining sample conditions from raw data with iterative hydrocode analysis

In some cases the particle velocity of the interface between sample and window cannot be obtained directly as strong shocks can transform the transparent window to an opaque material. In those instances only the free surface velocity can be obtained by the velocity diagnostics and an iterative Lagrangian analysis (ILA) must be used to determine the sound speed; stress-density information can then be calculated [4]. Using the ILA, the velocity-time history during the compression can be obtained from the free surface measurements and from knowledge of the optical laser pulse to x-ray pulse delay, the exact state probed by the x-ray is obtained.

In the same way that the velocity-time history of the sample can be obtained from rear-surface velocity ILA, the particle velocity measured at the interface can be used to iterate hydrocode laser pulse shapes such that the same velocity-time trace is obtained in the hydrocode. With knowledge of the x-ray probe timing (with respect to the optical laser), the exact condition within the sample during the x-ray probe time can be obtained from the hydrocode, allowing a more robust understanding of the samples state.

2.2 X-ray matter interaction

In the proposed experimental setup, discussed in detail further below, the shock compressed matter is diagnosed by X-ray Absorption Fine Structure (XAFS) spectroscopy and radiography. Both techniques can be modeled with appropriate simulation tools as described in the following.

The x-ray probe duration, during laser shock compression, can range from nanosecond down to femtosecond exposures. X-ray pulses for shock compression studies at the ESRF are ≈ 100 ps long. Table 2 lists the most important x-ray parameters.

[1] The Esther hydrocode is currently presented in French only.

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Photon energy	5 keV - 28 keV
Polarization	horizontal
Focus size (fwhm)	3 μm (5 keV) - 50 μm (28 keV)
Pulse length	100 ps
Flux	1×10^{14} photons/s (7 keV) - 4×10^{13} photons/s (28 keV)

Table 2: Principal x-ray parameters for shock compression studies at ESRF (beamline ID24)

2.3 XAFS

The XAFS signal reflects the near order of the shock compressed matter. The absorption edge is modulated by the ion-ion correlation function $\chi(\vec{q})$ making it possible to identify the crystalline structure in the absorption spectrum. XAFS can be simulated by combining first principle electronic structure methods with linear response theory. A well known implementation is the non-open source code FEFF [5].

2.4 Radiography

Standard radiography can be used to image e.g. the shock front during dynamical compression. The software Oasys [6], being a front-end to the ShadowOui raytracing software has the capability to calculate radiographs from simulated density profiles.

3 Experimental scenario

Fig. 1 shows the experimental setup, optical laser and x-ray probe pulse timings (a), measured XANES (x-ray absorption near edge spectroscopy) spectra (b) and 1D radiation-hydrodynamic simulations of shock propagation through the a sandwiched iron target. The figure is taken from Ref. [7]. The drive pulse compresses the target as modeled by radiation hydrodynamics simulations reaching pressures in the range of 40 – 60 GPa. The x-ray pulse of $\approx$ 100 ps probes the compressed target after a variable time delay. Transmitted x-ray photons are detected in a position sensitive Ge detector. The position of the detected photon can be converted into photon energy employing the dispersion curve of the focussing mirror.

4 Application: Pulse optimization via feedback loop

Radiation-hydrodynamic simulations are an indispensable tool to estimate the achievable level of compression and pressures in a dynamic compression experiment. Tailored (ramp) pulses can be employed to generate low-isentrope compressions, i.e. reaching high densities at low temperatures, below the principal Hugoniot and below the melting temperature. This technique makes accessible the range of strongly compressed solid matter and study pressure induced structural and electronic phase transitions.

To facilitate pre-shot simulations and pulse optimization, we will utilize the simulation capabilities of *simex_platform* inside an optimization loop (Fig. 2). Using an initial guess for the (temporal) pulse shape, we run the radiation-hydrodynamics simulations and monitor the evolution of density,

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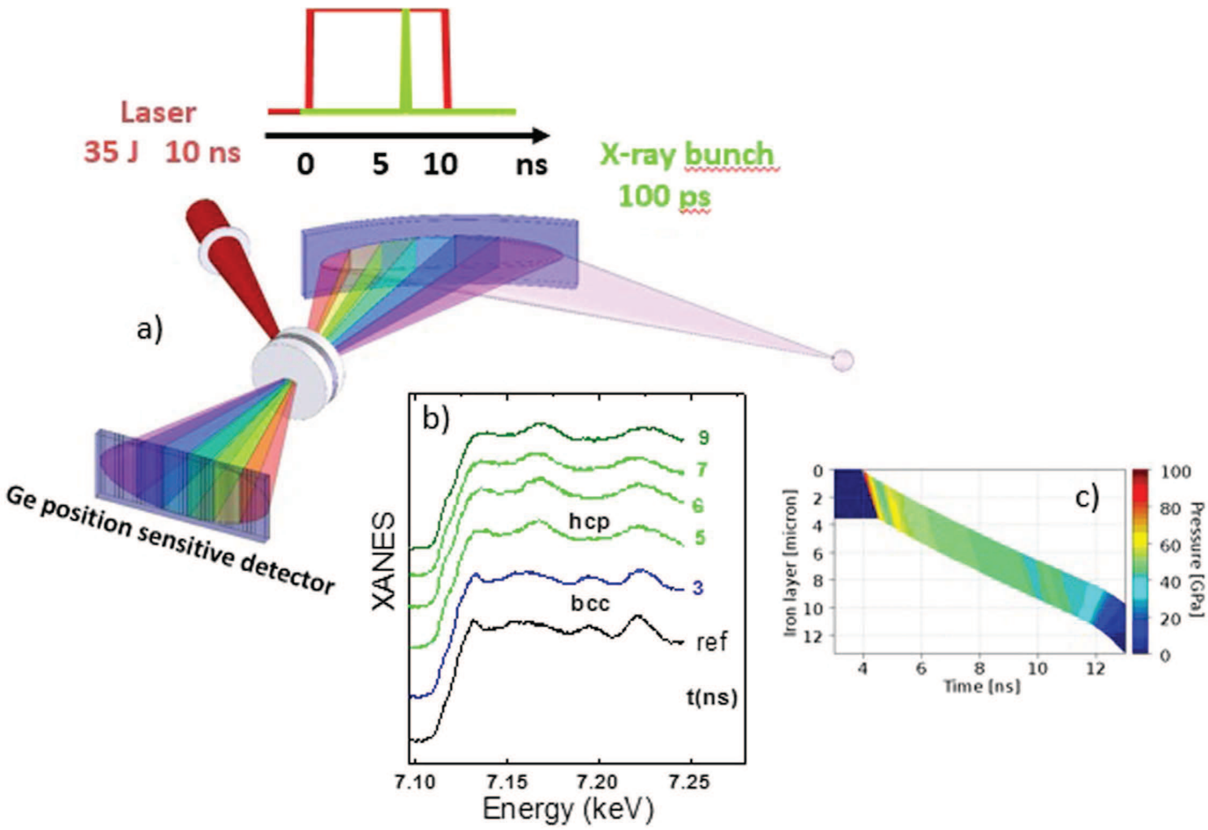

Figure 1: Schematic rendering of a laser driven shock compression experiment and x-ray absorption spectroscopy (a). XANES signal as function of time indicating structural phase transition from bcc to hcp phase (b). 1D Radiation-hydrodynamics simulation of the shock propagation and pressure dynamics during laser-matter interaction (c). Figure taken from Ref. [7].

pressure, and temperature over the pulse duration. This information is then fed to an algorithm that sets up a new, improved pulse shape based on given criteria like maximum allowable temperature or minimal compression ratio, to run the next iteration of the process. The pulse shaping tool can be implemented in various ways including nonlinear multidimensional optimization of pulse parameters or genetic algorithms.

5 Synergy

Although our pulse optimization scheme is independent of the technological and physical realization of pulse generation and control, it is desirable to incorporate the actual pulse generation mechanism, its capabilities as well as its limitations into the simulation workflow. This opens an opportunity for a cross-workpackage collaboration with the EUCALL workpackage 7 ("Pulse Control and ChAracterization – PUCCA")).

The development of an open data standard for radiation-hydrodynamics simulation is of high value for the scientific community also beyond EUCALL. It will facilitate integration of radiation-hydrodynamics codes into simulation frameworks such as `simex_platform`, benchmarking of vari-

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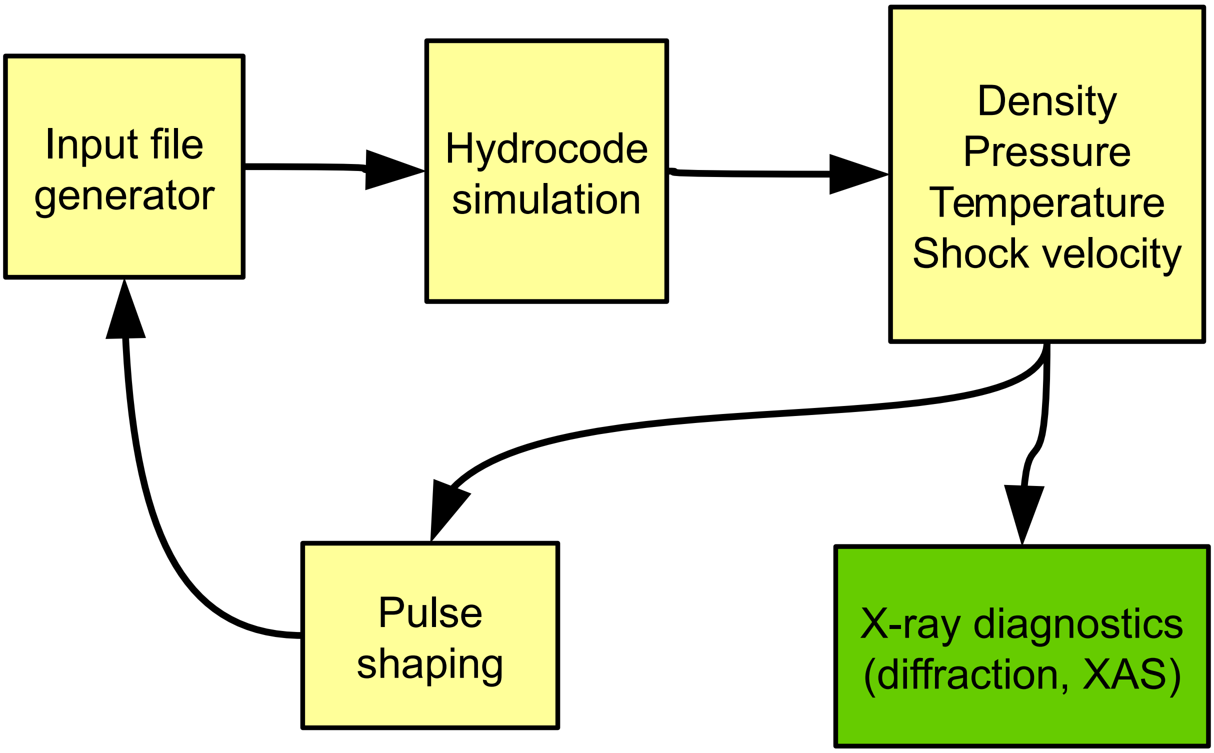

Figure 2: Optimization of pulse shapes for low isentrope compression. The output of radiation-hydrodynamics simulations is fed into a pulse shape generator to optimise the laser-matter interaction for maximum compression at low temperature increase. Once an optimized pulse is generated, the simulation continues with calculating the x-ray – matter interaction and synthesizing the diagnostic signals

ous codes against each other, against other methods (e.g. particle-in-cell simulations), and against experimental data.

6 Summary

We designed simulations of advanced laser matter-interaction in the context of warm dense matter research. WDM creation is simulated using radiation-hydrodynamics to predict the thermodynamic state of the target during the exposure. X-ray absorption and radiography diagnostics signal will be simulated within the `simex_platform` environment. A novel aspect is an iterative optimization scheme for pulse shape optimization to achieve low isentrope compression required to produce solids at extreme conditions of pressure and density at moderate temperatures below melting.

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References

1. Colombier, J. P., Combis, P., Bonneau, F., Harzic, R. L., and Audouard, E., *Hydrodynamic simulations of metal ablation by femtosecond laser irradiation*, *Phys. Rev. B* **71**, <http://dx.doi.org/10.1103/PhysRevB.71.165406> (2005).
2. Ramis, R., Meyer-ter-Vehn, J., and Ramírez, J., *MULTI2D - a computer code for two-dimensional radiation hydrodynamics*, *Computer Physics Communications* **180,** 977–994 (2009).
3. *openPMD Meta Data Format for Particle Mesh data*, <http://www.openpmd.org>.
4. Rothman, S. D., and Maw, J., *Characteristics analysis of isentropic compression experiments (ice)*, *J. Phys. IV. France,* 745–750 (2006).
5. Rehr, J. *et al.*, *Ab initio theory and calculations of X-ray spectra*, *Comptes Rendus Physique* **10,** 548–559 (2009).
6. Del Rio, M. S., Rebuffi, L., Demsar, J., N.Canestrari, and Chubar, O., *A proposal for an open source graphical environment for simulating X-ray optics*, *Proc. SPIE 9209,* 9209X (2014).
7. Torchio, R. *et al.*, *Probing local and electronic structure in Warm Dense Matter: single pulse synchrotron x-ray absorption spectroscopy on shocked Fe*, *Sci. Rep.* **6,** 26402 (2016).

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