# WP 4 – SIMEX

# Milestone M4.1: Delivery of individual simulation modules and common interfaces for interoperability

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# 1 Introduction

The computer program simex_platform [1] is a modular software environment for the simulation of experiments at advanced laser light sources. Users can assemble a virtual experiment through the combination of suitable simulation codes for the various instrumental parts of the experiment: the light source (e.g. a synchrotron, an x-ray free electron laser), propagation of radiation from the source to the point of interaction with a sample or target, interaction of the light with the sample, propagation of the scattered and transmitted light after the interaction, and detection. We have equipped simex_platform with a number of such codes and user interfaces to ease setup and execution of simulation runs. A lightweight abstraction mechanism and interface templates makes the integration of further simulation codes straightforward, so users can include their own or 3rd party simulation codes in the framework. In this way, they can embed their codes into a more realistic simulation environment compared to running codes isolated with more or less idealized parameters and initial conditions.

## 1.1 The EUCALL Software repository

The central access point for all codes, scripts, and documentation in SIMEX is the EUCALL software repository at https://github.com/eucall-software. The repository hosts the code for simex_platform at https://github.com/eucall-software/simex_platform next to a number of code projects for various simulation tasks, e.g. short-pulse laser matter interaction (https://github.com/eucall-software/picongpu) and coherent diffraction (https://github.com/eucall-software/singfel). The repository is also used for non-software collaborative projects, e.g. publication manuscripts and presentations.

## 1.2 Modular structure of virtual photon experiments and simulation *Calculators*

In its current state, simex_platform supports simulation of photon experiments, that follow a linear base pattern: The radiation is produced from a photon source, propagated through a beamline, it interacts with a sample (target), and photons leaving the sample after scattering or emission are detected in a photon detector. This linear progression, depicted in Fig. 1, will be referred to as the simulation baseline in the following. A typical example is a x-ray diffraction experiment: X-ray photons delivered by a synchrotron or an FEL, scatter from a sample (e.g. a

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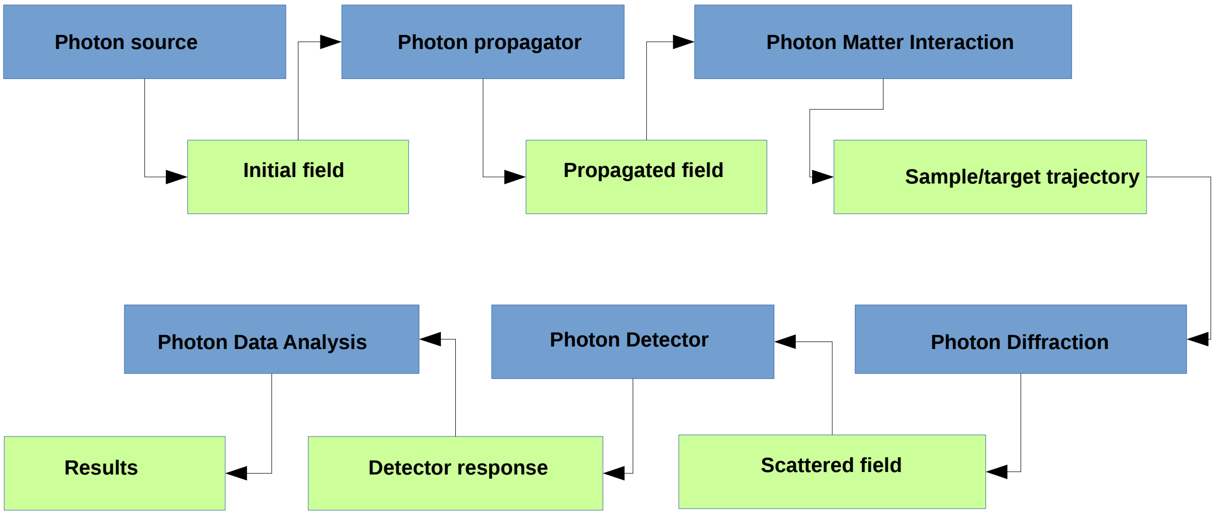


Figure 1: Baseline workflow in `simex_platform`. Blue boxes represent *Calculators*, green boxes are data interfaces.

crystal), and diffracted photons are captured in an area detector behind the sample. Other baseline applications are e.g. small and wide angle scattering, inelastic x-ray scattering, or x-ray absorption spectroscopy. Simulation of experiments in `simex_platform` that are not directly representable in this ordered linear pattern are possible but not supported in the same way and to the same extent as baseline applications. For example, experiments that involve more than one photon source, or applications where products from photon-matter interaction (e.g. accelerated electrons or ions) are required for further interactions, such as laser-plasma based short pulse length x-ray and UV sources, proton radiography and cancer therapy using laser accelerated protons.

A baseline application encapsulates five parts: The photon source, the photon transport from the source to the experiment, the interaction of photons and matter, propagation of scattered and transmitted radiation from the target/sample to the detector, and photon detection. In `simex_platform` each of these blocks is represented by a suitable *Calculator*. A *Calculator* can be seen as an operator acting on the data representing radiation. It reads data from an input, performs a calculation with the data, potentially modifies the data based on the calculation results, and writes the modified or propagated radiation to its output. Calculators are organized in a lightweight abstraction scheme, represented in Fig. 2.

Commonalities between calculators are implemented on higher levels of abstraction (blue or yellow boxes) whereas specialities of each individual *Calculator* are encapsulated in the derived classes (green boxes). By providing as much func-

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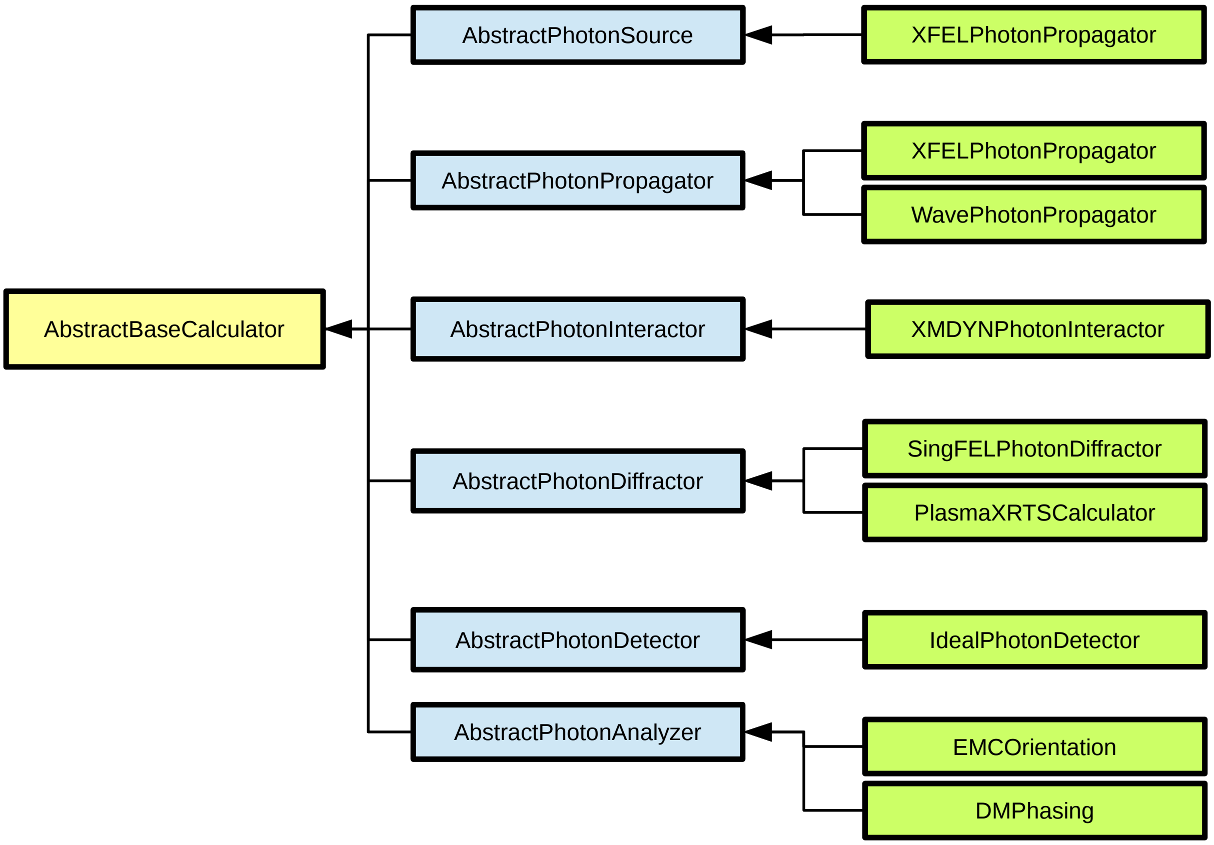


Figure 2: Inheritance tree for *Calculators* in `simex_platform`.

tionality as possible on the abstract level, the task of adding a new calculator to the set of existing calculators is facilitated to a large degree, making `simex_platform` user friendly and opening collaborative opportunities, also beyond EUCALL.

## 1.3 Interfaces

Start-to-end simulations in `simex_platform` require that any two subsequent *Calculators* employed in the simulation pipeline can communicate data amongst each other. The data source has to write the data in a format that the ensuing data sink can handle and interpret correctly. In `simex_platform`, we chose the Hierarchical Data Format (hdf5) [2] as the underlying format for all simulation data files. Data consistency in the workflow is realized by each *Calculator* defining the names of hdf datasets and attributes that it requires to perform its calculation task and the names of all datasets and attributes that it provides to the subsequent calculator. In this way, after instantiating the *Calculators* for a simulation, the user or a workflow manager can check if the data can be channeled through the *Calculators* and

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give a feedback if there is a mismatch between provided and expected data for two subsequent *Calculators*. This approach is inherited from the preceding simulation framework `simS2E` [3, 4]. Recently, we have started to adopt a more general approach of defining inter-calculator interfaces based on the open standard for particle-mesh data `openPMD` (`www.openpmd.org`).

### 1.4 Backengines

The *Calculators* in `simex_platform` are user interfaces to software executables or scripts that perform the actual mathematical operations on the *Calculator's* input data. In the following, we refer to these executables and scripts as the *Backengines*. One *Calculator* always wraps exactly one *Backengine*, but one *Backengine* can be wrapped by more than one *Calculator*.

## 2 Baseline science applications and required simulation codes

An intermediate goal in SIMEX is to enable simulation of three distinct baseline experiments. The following tables list the simulation codes (*backengines*) that will be employed for the simulation, as well as relevant references and links to further details. The linked sections give a brief description of the numerical and physical methods and specify the data interfaces.

1. Single-particle imaging at the European XFEL (SPB-SFX instrument)

| Module | Backengine | References | Details |
|---|---|---|---|
| Photon source | FAST, XPD database | [5, 6] | 3.1.1 |
| Propagation | WPG/SRW | [7, 8] | 3.2.1 |
| Photon-Matter Interaction | XMDYNandXATOM | [9, 10, 11] | 3.3.1 |
| Photon diffraction | singFEL | [3] | 3.3.5 |
| Photon detection | X-CSIT | [12] | 3.4.1 |

2. Small-angle x-ray scattering from high power laser excited overdense plasmas (XFEL, HED instrument)

| Module | Backengine | References | Details |
|---|---|---|---|
| Photon source | FAST, XPD database | [5, 6] | 3.1.1 |
| Propagation | WPG/SRW | [7, 8] | 3.2.1 |
| Photon-Matter Interaction | PIConGPU | [13] | 3.3.2 |
| Photon scattering | paraTAXIS | [14] | 3.3.4 |
| Photon detection | X-CSIT | [12] | 3.4.1 |

3. Warm dense matter production through high energy laser shock compression and x-ray radiography diagnostics (ESRF, beamline ID24)

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| Module | Backengine | References | Details |
|---|---|---|---|
| Propagation | Oasys/ShadowUI | [15] | 3.2.2 |
| Photon-Matter Interaction | Esther, Multi2D | [16, 17] | 3.3.3 |
| Radiography | Oasys/ShadowOui | [15] | 3.2.2 |

# 3 Listing of SIMEX *Backengines*, and interfaces

This section gives more detailed information about the simulation codes used in SIMEX, their data interfaces as well as graphical representations of simulation data to demonstrate their functionality.

## 3.1 Photon source

### 3.1.1 FAST

**Method:** 3D time resolved explicit solver

**Domain:** SASE FEL simulation

**Data structure:**

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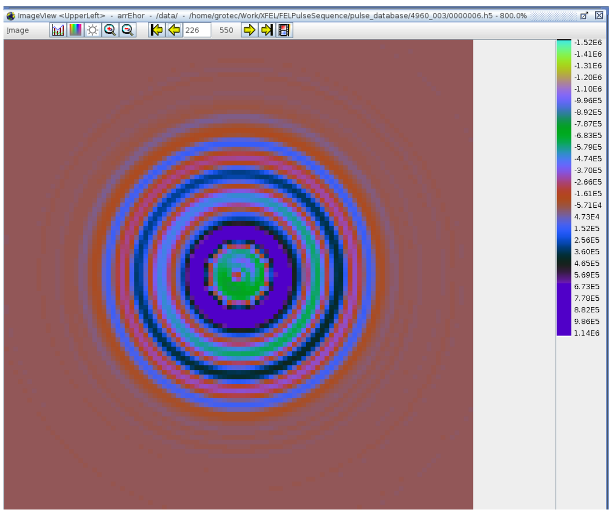
| | |
|---|---|
| /data/arrEhor | horizontal electric field component |
| /data/arrEver | vertical electric field component |
| /params/Mesh/nSlices | number of time slices |
| /params/Mesh/nx | number of grid points in horizontal dimension (x) |
| /params/Mesh/ny | number of grid points in vertical dimension (y) |
| /params/Mesh/sliceMax | time corresponding to last slice |
| /params/Mesh/sliceMin | time corresponding to first slice |
| /params/Mesh/xMax | x coordinate of last grid point in horizontal dimension |
| /params/Mesh/xMin | x coordinate of first grid point in horizontal dimension |
| /params/Mesh/yMax | y coordinate of last grid point in vertical dimension |
| /params/Mesh/yMin | y coordinate of first grid point in vertical dimension |
| /params/Mesh/zCoord | z coordinate of the wavefront |
| /params/Rx | instantaneous horizontal wavefront radius |
| /params/Ry | instantaneous vertical wavefront radius |
| /params/dRx | error in Rx |
| /params/dRy | error on Ry |
| /params/nval | data type of field values, 2 for complex |
| /params/photonEnergy | central photon energy (mean of spectrum) |
| /params/wDomain | time or frequency domain |
| /params/wEFieldUnit | Electric field unit |
| /params/wFloatType | field numerical type |
| /params/wSpace | direct (r-space) or reciprocal (q-space) |
| /params/xCentre | x coordinate of wavefront center |
| /params/yCentre | y coordinate of wavefront center |
| /history/parent/info/data_description | data documentation |
| /history/parent/info/package_version | code version |
| /history/parent/misc/FAST2XY.DAT | |
| /history/parent/misc/angular_distribution | angular distribution of source pulse |
| /history/parent/misc/spot_size | fhwm spot size |
| /history/parent/misc/gain_curve | gain curve |
| /history/parent/misc/nzc | Undulator length (point on gain curve0 |
| /history/parent/misc/temporal_struct | Temporal pulse structure (on-axis projection) |

## Example data:



FEL source calculation using the code FAST: Horizontal component of electric field distribution near pulse center in a plane perpendicular to propagation direction at undulator exit in SASE 1 beamline at the European XFEL [6].

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## 3.2 Photon Propagation (Task 4.1.1)

Propagates the radiation as described by the photon source calculator from the source to the point of interaction with the sample or target under investigation. Describes focussing, filtering, pulse shaping, and other optical effects realized through lenses, mirrors, apertures, grids etc.

### 3.2.1 WPG/SRW

**Method:** Fourier optical wave propagation

**Data structure:**

| | |
|---|---|
| /data/arrEhor | horizontal electric field component |
| /data/arrEver | vertical electric field component |
| /params/Mesh/nSlices | number of time slices |
| /params/Mesh/nx | number of grid points in horizontal dimension (x) |
| /params/Mesh/ny | number of grid points in vertical dimension (y) |
| /params/Mesh/qxMax | x coordinate of last q-grid point in horizontal dimension |
| /params/Mesh/qxMin | x coordinate of first q-grid point in horizontal dimension |
| /params/Mesh/qyMax | y coordinate of last q-grid point in vertical dimension |
| /params/Mesh/qyMin | y coordinate of first q-grid point in vertical dimension |
| /params/Mesh/sliceMax | time corresponding to last slice |
| /params/Mesh/sliceMin | time corresponding to first slice |
| /params/Mesh/xMax | x coordinate of last grid point in horizontal dimension |
| /params/Mesh/xMin | x coordinate of first grid point in horizontal dimension |
| /params/Mesh/yMax | y coordinate of last grid point in vertical dimension |
| /params/Mesh/yMin | y coordinate of first grid point in vertical dimension |
| /params/Mesh/zCoord | z coordinate of the wavefront |
| /params/Rx | instantaneous horizontal wavefront radius |
| /params/Ry | instantaneous vertical wavefront radius |
| /params/dRx | error in Rx |
| /params/dRy | error on Ry |
| /params/nval | data type of field values, 2 for complex |
| /params/photonEnergy | central photon energy (mean of spectrum) |
| /params/wDomain | time or frequency domain |
| /params/wEFieldUnit | Electric field unit |
| /params/wFloatType | field numerical type |
| /params/wSpace | direct (r-space) or reciprocal (q-space) |
| /params/xCentre | x coordinate of wavefront center |
| /params/yCentre | y coordinate of wavefront center |
| /info/package_version | WPG version |
| /info/contact | Support contact details |
| /info/data_description | Data documentation |
| /info/method_description | Method documentation |
| /misc/xFWHM | Full width at half maximum of the intensity distribution in horizontal dimension |
| /misc/yFWHM | Full width at half maximum of the intensity distribution in vertical dimension |
| /version | Interface version |

**Example data:**

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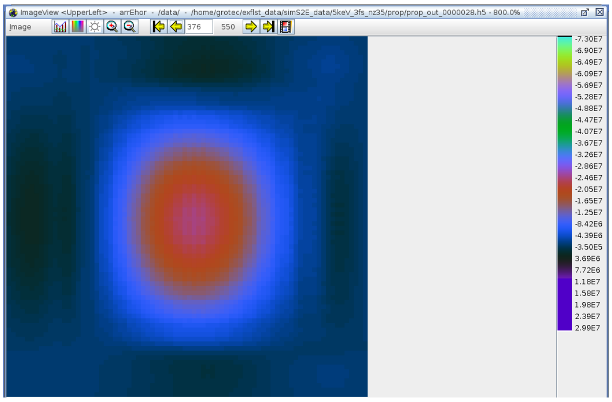

Propagation of source wavefront as calculated by WPG: Horizontal component of electric field distribution near pulse center in plane perpendicular to propagation direction at sample position in the SPB-SFX instrument at European XFEL.

### 3.2.2 Oasys

**Method:** X-ray raytracing

**Domain:** Synchrotron radiation propagation

**Data structure:** See Ref. [15]

**Example data:** See Ref. [15]

## 3.3 Photon Interactor (Task 4.1.2)

Interaction of the photons with the target or sample. Takes into account elementary processes like absorption, emission, scattering of radiation and secondary processes like collisional ionization and recombination. The end product is the electronic state of the sample/target as a function of time during the interaction with the external light source.

### 3.3.1 XMDYNandXATOM

**Method:** Molecular Dynamics and Hartree-Fock electronic structure

**Domain:** Atoms and Molecules in intense x-ray fields

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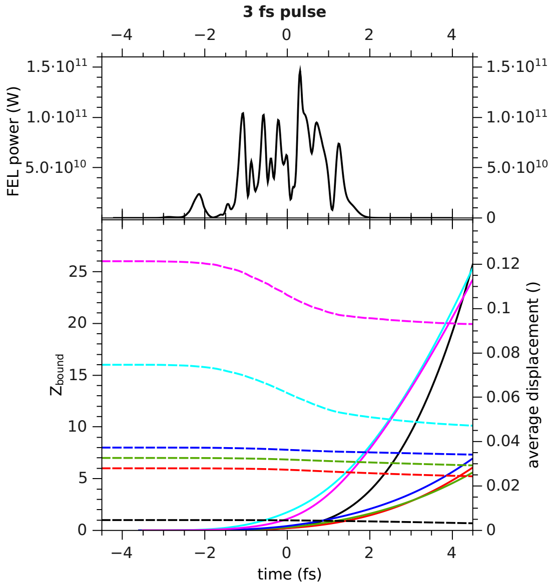
**Data structure:**

| | |
|---|---|
| /data/snp*/ff | 2D array of form factors. Rows: Atomic number, Columns: q |
| /data/snp*/halfQ | 1D array of half-period resolutions corresponding to column index in form factor arrays |
| /data/snp*/Nph | number of photons in the calculation |
| /data/snp*/r | 2D array of atomic position vectors. Rows: Atom index, columns: x,y,z coordinates |
| /data/snp*/T | 1D array of unique ID per atomic number |
| /data/snp*/Z | 1D array of atom types per atomic position vector *r* |
| /data/snp*/xyz | 1D array of indices of ff for each atom in Z |
| /data/snp*/Sq_halfQ | half period resolution q space spanned by Sq_bound, Sq_free |
| /data/snp*/Sq_bound | 1D array for Compton scattering from bound electrons |
| /data/snp*/Sq_free | 1D array for Compton scattering from free electrons |
| /history/parent/detail | Input parameters used to run the code |
| /info/package_version | backengine code version |
| /info/contact | Support contact for backengine code |
| /info/data_description | Data documentation |
| /info/method_description | Method documentation |
| /version | hdf5 format version |

**Example data:**




Photon-matter calculation using XMDYNandXMATOM: 3 fs XFEL pulses (5 keV photon energy) (power vs time, top panel), average displacement, and average ionization (bottom) [18] for the irradiated 2NIP molecule [19]. This figure was published in Ref. [20].

### 3.3.2 PIConGPU

**Method:** 3D3V Particle-In-Cell (PIC)

**Data structure:** openPMD incl. domain extension for PIC.

**Example data:**

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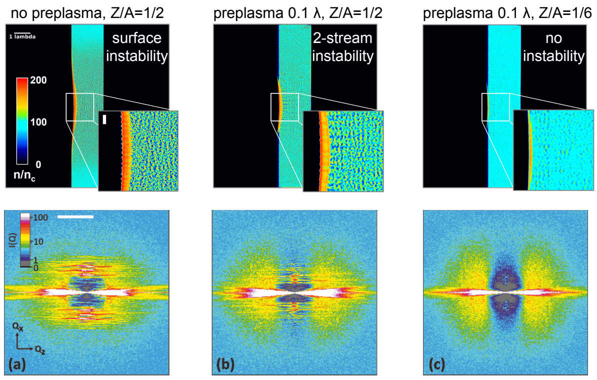



PIConGPU calculations of electron density (top) and corresponding Small Angle X-ray Scattering signals (bottom) from high power laser – matter interaction.

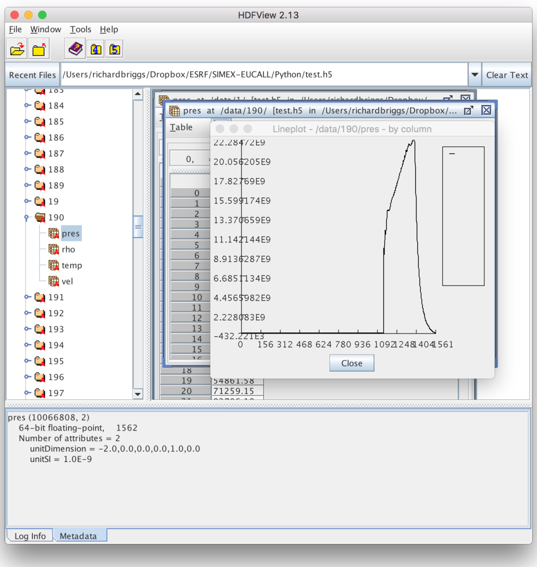
### 3.3.3 Esther

**Method:** 1-D radiation hydrodynamics

**Domain:** Dynamic compression

**Data structure:** openPMD

**Example data:**




Shock front simulation using Esther: Pressure vs. distance after high energy – solid matter (iron) interaction.

### 3.3.4 paraTAXIS

**Method:** MonteCarlo tracking of individual photons

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**Domain:** Ex-situ and in-situ photon scattering from strongly excited plasmas

**Data structure:** openPMD particles

**Demonstraction data:** See 3.3.2

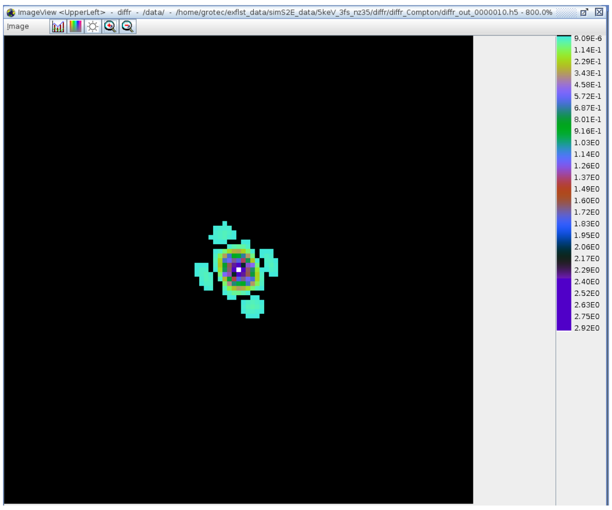
### 3.3.5 singFEL

**Method:** 2nd order Born approximation scattering using electronic form factors.

**Data structure:**

| | |
|---|---|
| /data/data | 2D array. Integrated intensity per pixel |
| /data/diffr | 2D array. Integrated intensity converted to photon count (Poissonized) |
| /data/angle | Euler angles applied to atomic positions |
| /history/parent/detail | Details of parent data |
| /history/parent/parent | Parent data, hierarchical |
| /info/package_version | Backengine code version |
| /info/contact | Support contact |
| /info/data_description | Data documentation |
| /info/method_description | Method documentation |
| /params/geom/detectorDist | Detector distance |
| /params/geom/pixelWidth | Pixel width (x) |
| /params/geom/pixelHeight | Pixel height (y) |
| /params/geom/mask | Masked pixels |
| /params/beam/photonEnergy | Central photon energy |
| /params/beam/photons | Number of photons in beam |
| /params/beam/focusArea | Beam focus area |
| /params/info | Input parameter for backengine code |

**Example data:**



Simulated diffraction intensity distribution using singFEL.

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### 3.3.6 XRTS code

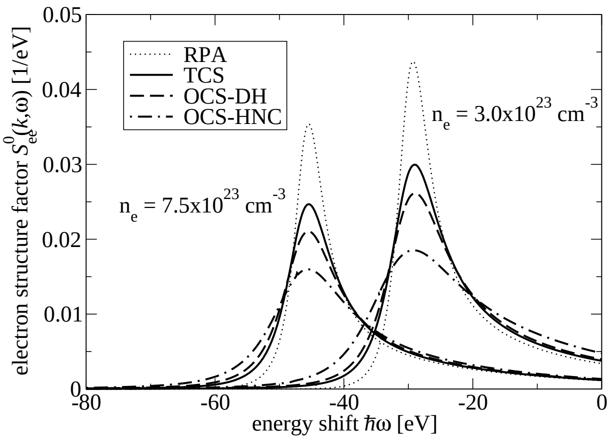
**Method:** 2nd Born approximation for differential inelastic scattering cross section for scattering from warm and hot dense plasmas in various approximations [21, 22, 23]

**Domain:** X-ray Thomson Scattering in Dense Plasmas

**Data structure:**

| | |
|---|---|
| /data/dynamic/Skw_bound | Bound electron Compton scattering structure factor |
| /data/dynamic/Skw_free | Free electron scattering structure factor |
| /data/dynamic/Skw_total | Total scattering structure factor |
| /data/dynamic/energy_shifts | Range of energy shifts spanned by dynamic structure factors |
| /data/static/Sk_core | Core electron static structure factor |
| /data/static/Sk_free | Free electron static structure factor |
| /data/static/Sk_ion | Ion static structure factor |
| /data/static/Sk_total | Total static structure factor |
| /data/static/Wk | Ion feature $\|f+q\|^2 S_{ii}(k)$ |
| /data/static/debye_waller | Debye-Waller factor |
| /data/static/fk | Atomic form factor $f(k)$ |
| /data/static/ipl | Ionization potential lowering |
| /data/static/lfc | Local field factor |
| /data/static/qk | Screening cloud $q(k)$ |

**Example data:**




Simulated X-ray Thomson Scattering spectra using various ion-ion structure factor models for two electron densities. Scattered intensity as function of energy shift, simulated with XRTS code.

## 3.4 Photon Detector (Task 4.1.4)

### 3.4.1 X-CSIT

**Method:** Combined particle, charge, and electronics simulation

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**Domain:** Pixel area detectors

**Data structure:**

| | |
|---|---|
| /data/diffr | 2D array. Photon count per pixel (Poissonized) |
| /history/parent/detail | Details of parent data |
| /history/parent/parent | Parent data, hierarchical |
| /info/package_version | Backengine code version |
| /info/contact | Support contact |
| /info/data_description | Data documentation |
| /info/method_description | Method documentation |
| /params/geom/detectorDist | Detector distance |
| /params/geom/pixelWidth | Pixel width (x) |
| /params/geom/pixelHeight | Pixel height (y) |
| /params/geom/mask | Masked pixels |
| /params/beam/photonEnergy | Central photon energy |
| /params/beam/photons | Number of photons in beam |
| /params/beam/focusArea | Beam focus area |
| /params/info | Input parameter for backengine code |

**Example data:** See Ref. [12].

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