# SIMulation of EXperiments

Carsten Fortmann-Grote

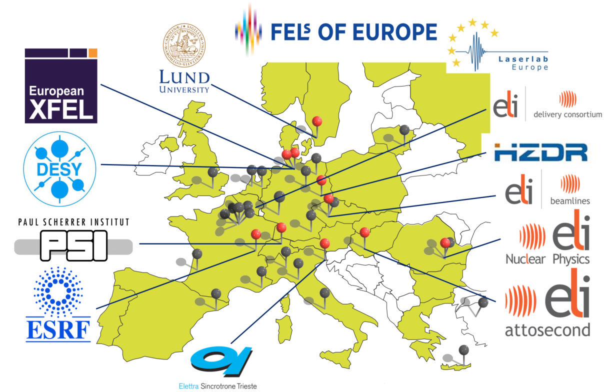
This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 654220

11'TH NOBUGS | 2016
Copenhagen, Denmark, 17th to 19th October
NEW OPPORTUNITIES FOR BETTER USER GROUP SOFTWARE

# EUropean Cluster of Advanced Laser Light Sources

## EUCALL is a network between large-scale user facilities for:

- free electron laser radiation
- synchrotron radiation
- optical laser radiation




## EUCALL researchers collaborate on:

- common methodologies and research opportunities
- tools to sustain this interaction in the future

## Facts and figures:

- 7M€ from Horizon 2020 for project period 2015 - 2018
- 11 partners from nine countries and two further clusters

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# Work packages

- WP1 – **Management** of the EUCALL Project
- WP2 – **Dissemination** and Outreach
- WP3 – **Synergy** of Advanced Laser Light Sources

- WP4 – **SIMEX**: Simulation of Experiments
- WP5 – **UFDAC**: Ultrafast Data Acquisition
- WP6 – **HIREP**: High Repetition Rate Sample Delivery
- WP7 – **PUCCA**: Pulse Characterisation and Control

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# The SIMEX team

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# Outline

- SIMEX objectives
- simex_platform: an opensource platform for simulation of photon experiments
  - Generic interfaces to advanced simulation codes
  - Open standards for data exchange
  - Supported baseline applications
- Science case: Single Particle Imaging at EU.XFEL
- Summary & Outlook

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# SIMEX' objective

The key objective of **SIMEX** is to develop and implement a simulation platform for users and facility operators to fully simulate experiments at the various light sources.

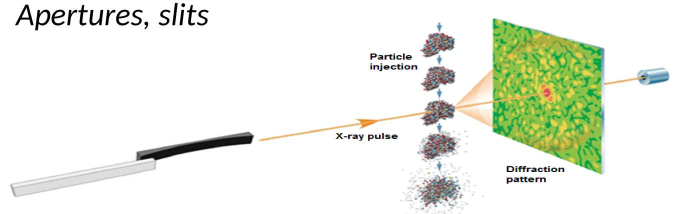
***Target/Sample***
- *Atoms, molecules, clusters*
- *Solids, surfaces*
- *Liquids*
- *Plasmas*

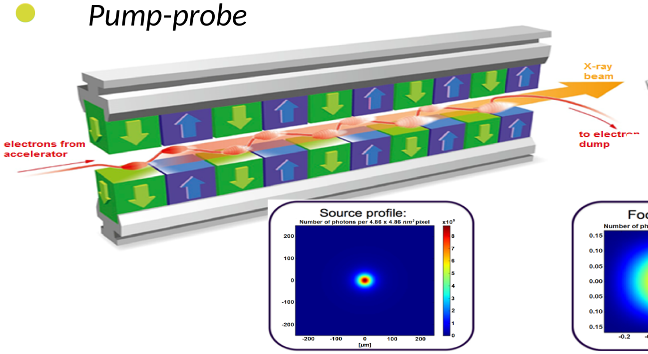
***Photon Data Analysis***
- *Structure determination*
- *Electronic structure*
- *Transport*
- *Relaxation & Thermodynamics*

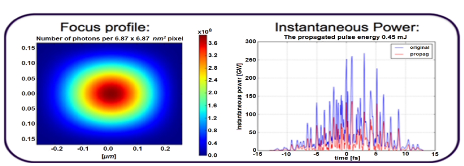
***Diagnostics***
- *Spectroscopy*
- *Diffraction*
- *Scattering*

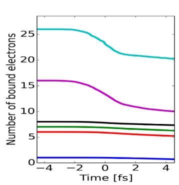
***Photon propagation***
- *Lenses*
- *Mirrors*
- *Apertures, slits*

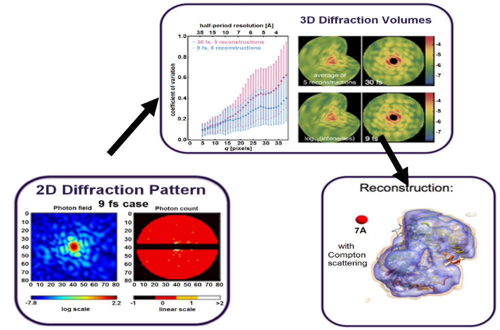
***Photon Source***
- *XFEL*
- *Synchrotron*
- *Optical Laser*
- *Pump-probe*

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# Some highlights about simex_platform

- Modular simulation platform for source-to-detector simulations in photon science
- Open source (www.github.com/eucall-software/ )
- Interfaces for various photon-matter interaction codes ready
- Various deployment options: Makefile, binaries, and Docker containers
- Performance boosts for 3rd party simulation codes

→Talk by S. Yakubov

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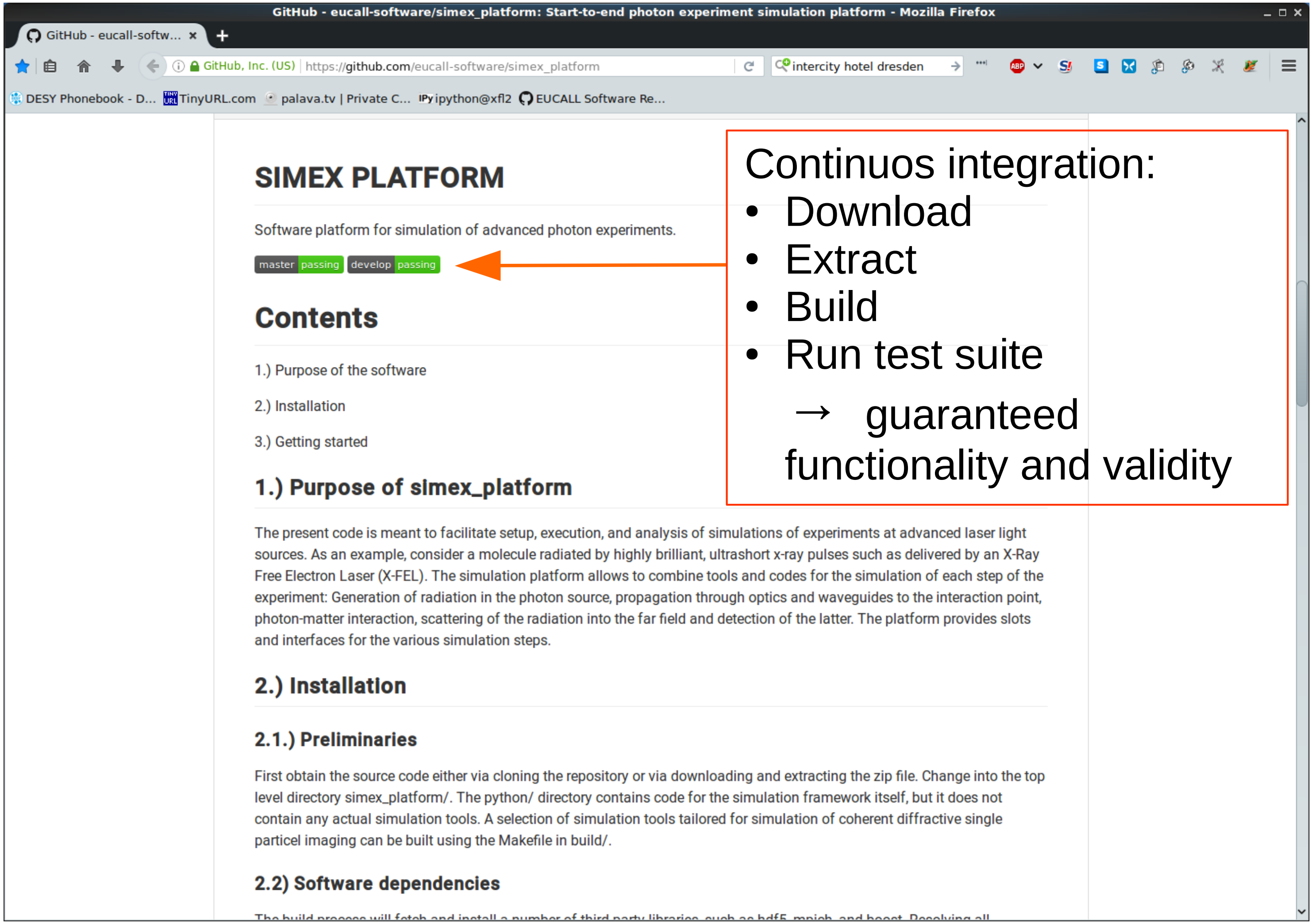
# SIMEX platform is on github


GitHub - eucall-software/simex_platform: Start-to-end photon experiment simulation platform - Mozilla Firefox

GitHub - eucall-softw... ×

GitHub, Inc. (US) | https://github.com/eucall-software/simex_platform

intercity hotel dresden

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## SIMEX PLATFORM

Software platform for simulation of advanced photon experiments.

master passing develop passing

## Contents

1.) Purpose of the software

2.) Installation

3.) Getting started

### 1.) Purpose of simex_platform

The present code is meant to facilitate setup, execution, and analysis of simulations of experiments at advanced laser light sources. As an example, consider a molecule radiated by highly brilliant, ultrashort x-ray pulses such as delivered by an X-Ray Free Electron Laser (X-FEL). The simulation platform allows to combine tools and codes for the simulation of each step of the experiment: Generation of radiation in the photon source, propagation through optics and waveguides to the interaction point, photon-matter interaction, scattering of the radiation into the far field and detection of the latter. The platform provides slots and interfaces for the various simulation steps.

### 2.) Installation

#### 2.1.) Preliminaries

First obtain the source code either via cloning the repository or via downloading and extracting the zip file. Change into the top level directory simex_platform/. The python/ directory contains code for the simulation framework itself, but it does not contain any actual simulation tools. A selection of simulation tools tailored for simulation of coherent diffractive single particel imaging can be built using the Makefile in build/.

#### 2.2) Software dependencies

Continuos integration:

- Download
- Extract
- Build
- Run test suite

→ guaranteed functionality and validity

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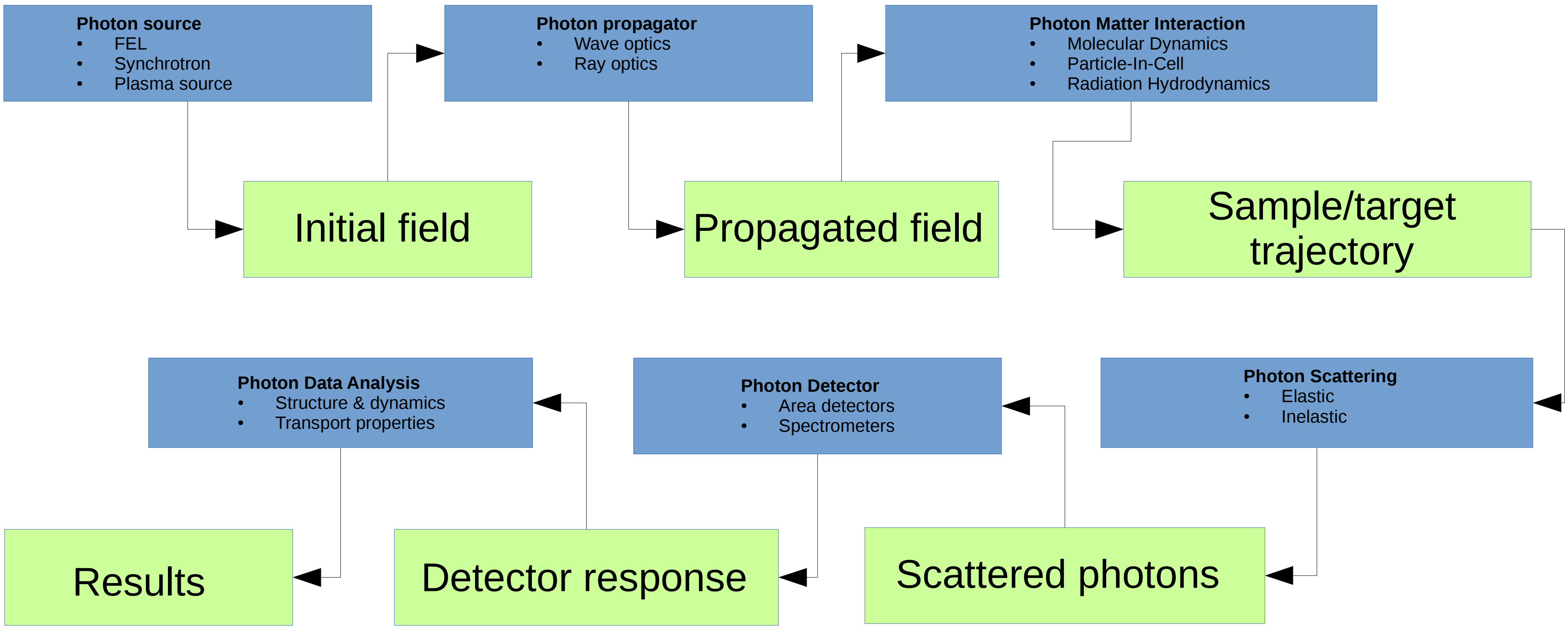
# Calculators and Interfaces in simex_platform

**Calculators**: Simulation codes + User interface (command line, py script)

**Interfaces**: hdf5 file + format description (simS2E, openPMD)

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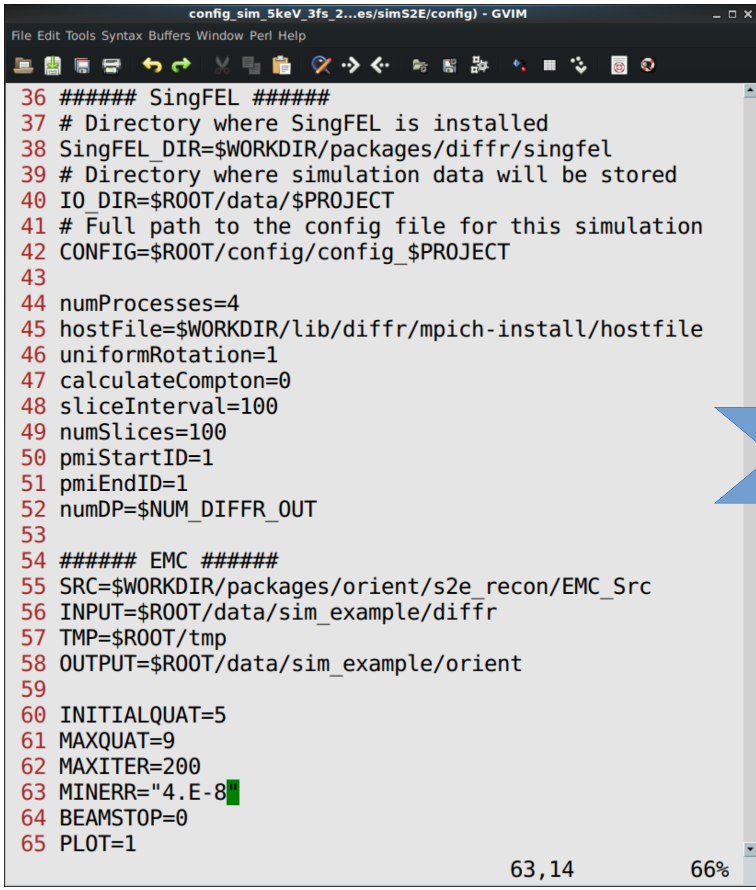
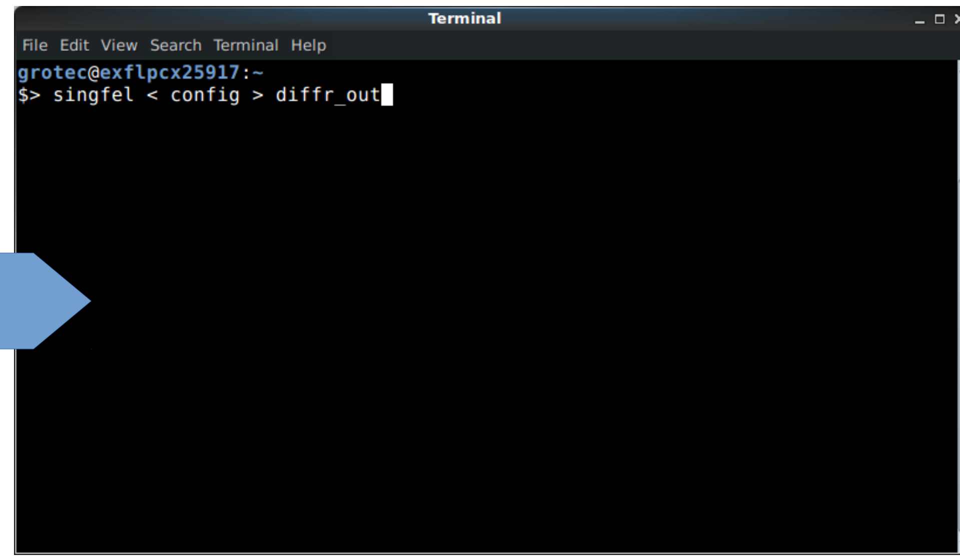
# User interface: from input decks ...




simS2E → Yoon et al. Science Rep. (2016)

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# … to Calculators

3fs_emc.py (~/Work/XFEL/SPB_3fs/reconstruction) - GVIM

```python
# Setup diffraction parameters. Some values are set to defaults.
diffraction_parameters = SingFELPhotonDiffractorParameters(
        uniform_rotation = True,
        calculate_Compton = True
        number_of_patterns = 20,
        slice_interval = 20,
        number_of_slices = 100)

# Change pmi_start_ID from default value.
diffraction_parameters.pmi_start_ID = 10

# Setup the diffraction calculator.
diffractor = SingFELPhotonDiffractor(parameters=diffraction_parameters)

# Can still change a parameter.
diffraction_parameters.parameter.pmi_stop_ID = 90

# Setup EMC parameters the old way.
emc_parameters={'max_number_of_quaternions'     : 9,
                'max_number_of_iterations'      : 100,
                'min_error'                     : 1.0e-8,
                'beamstop'                      : True,
                'detailed_output'               : True
               }

# Setup EMC calculator.
emc = EMCOrientation(parameters=emc_parameters)

# Run backengines.
status = True
while (status):
    status = diffractor.backengine()
    status = emc.backengine()

    break

# Get results.
emc_data = emc.data

# Center slice.
cslice = emc_data[:,:,50]

# etc.
```

Terminal

```
grotec@exflpcx25917:~
$> python diffr_emc.py
```

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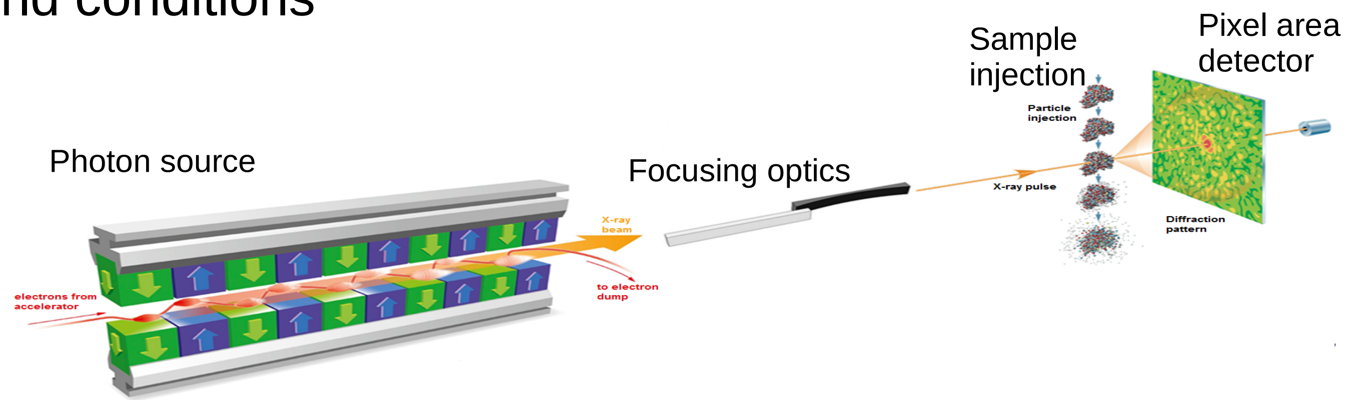
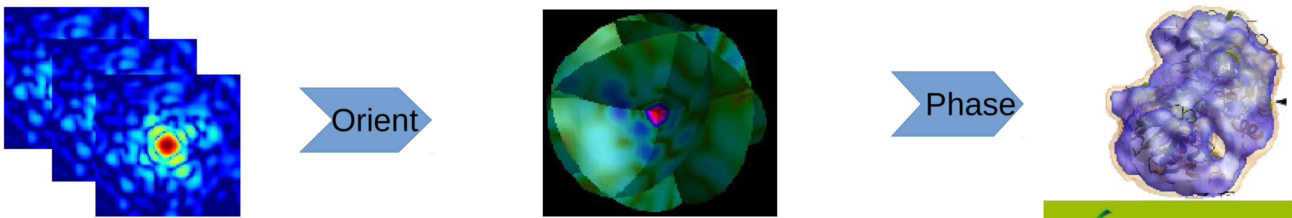
# Baseline science application #1: SPI

## Single Particle Imaging (SPI) at X-FELs

- Understand role of radiation damage processes using ab-initio simulations of photon-matter interaction (XMDYN & XATOM)
- Study effect of XFEL pulse properties on signal quality
- Benchmark and profile computational lensing algorithms under real-world conditions




Baseline setup

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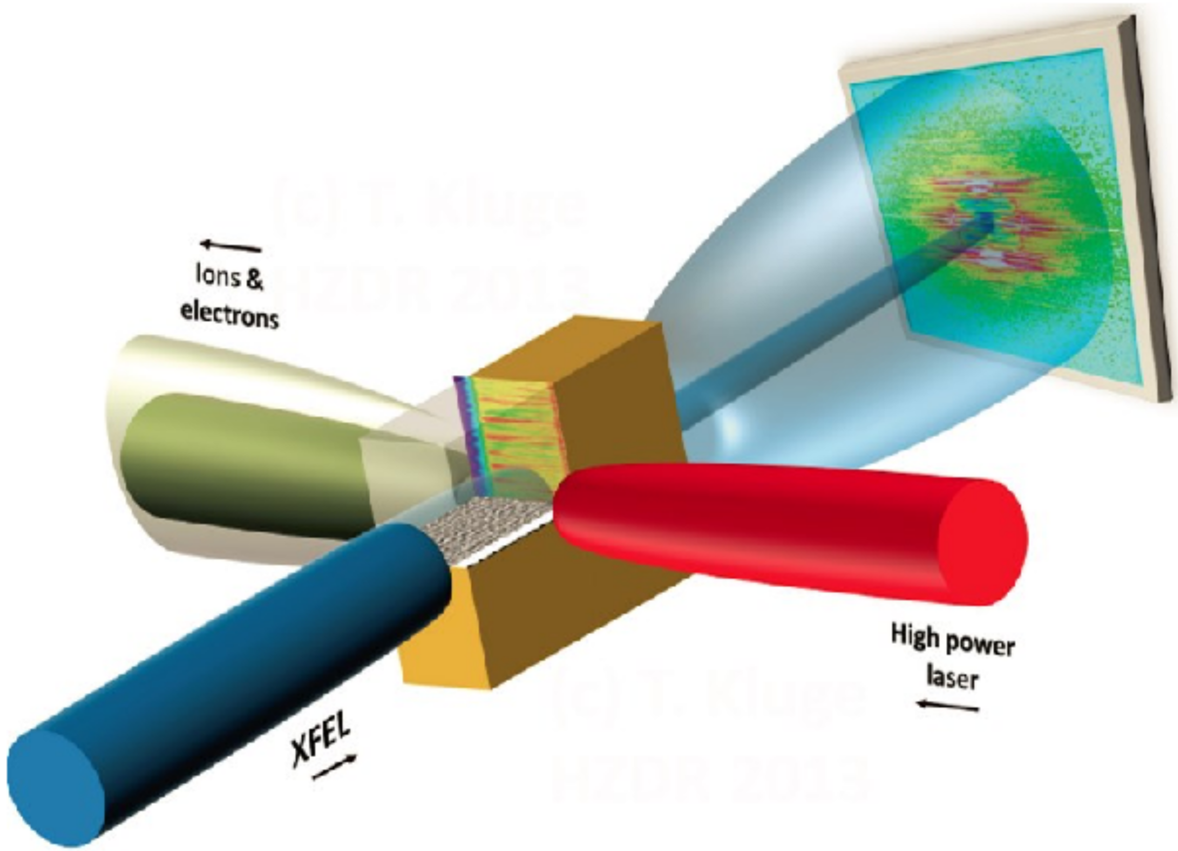
# Baseline science application #2: HPL

HZDR
HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

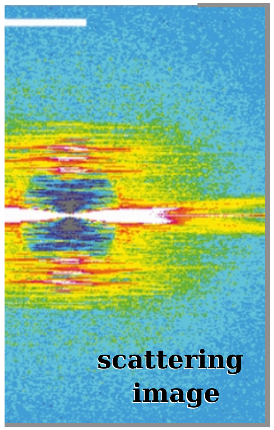
**X-ra**

- M ... ited
  p
- C
- E

Example Setup for Probing of Ultrafast Laser-Matter Interaction




XFEL beamli

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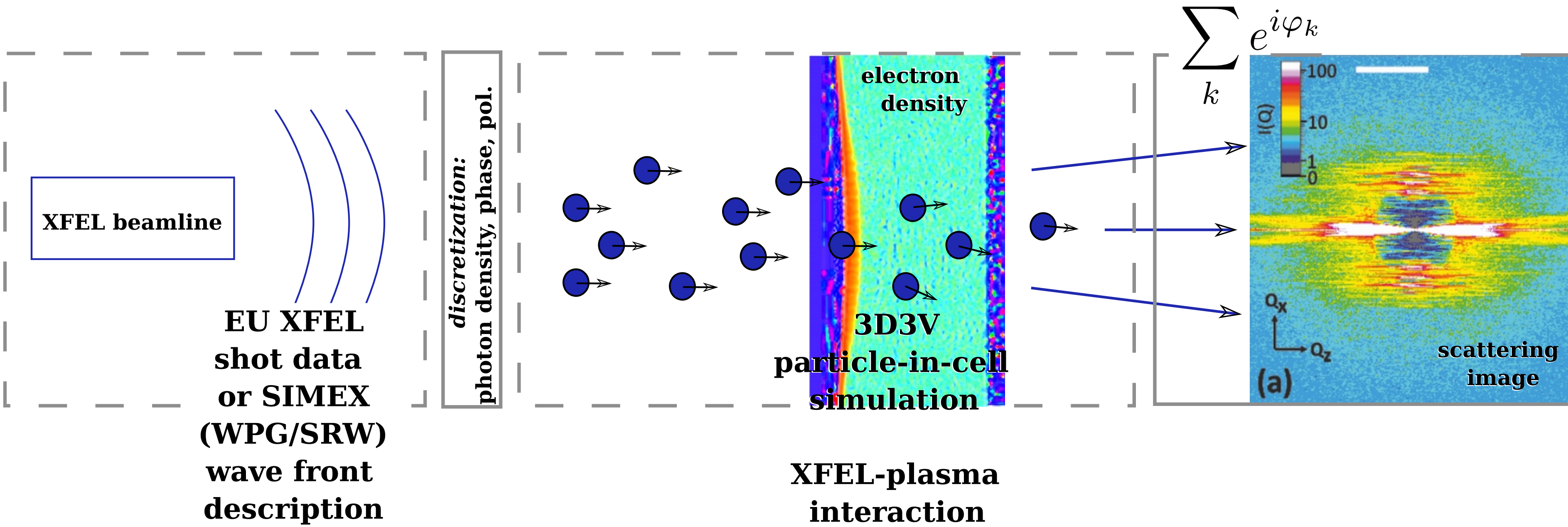
European XFEL

# Baseline science application #2: HPL

## X-ray probing of high power laser (HPL) excited matter

- Model non-equilibrium dynamics of ultrashort pulse laser excited plasmas with 3D3V Particle-In-Cell code PIConGPU
- Characterization of plasma instabilities via SAXS/WAXS
- Early science proposal for HED instrument at XFEL

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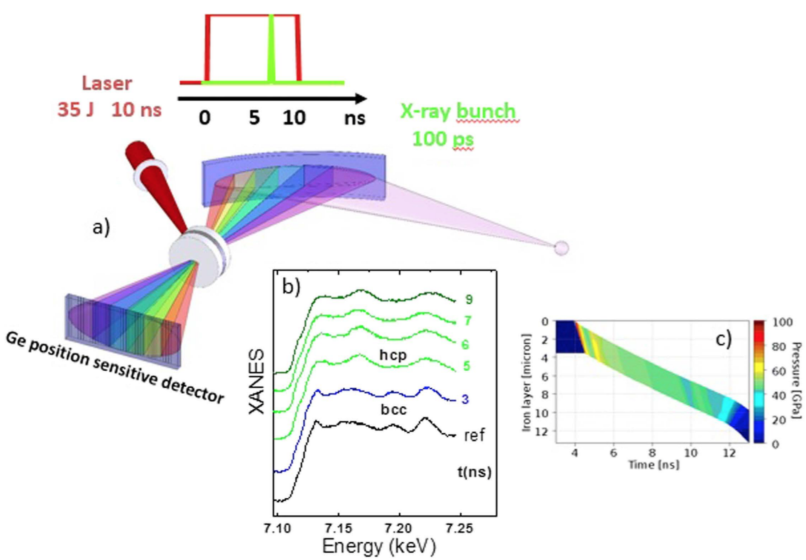
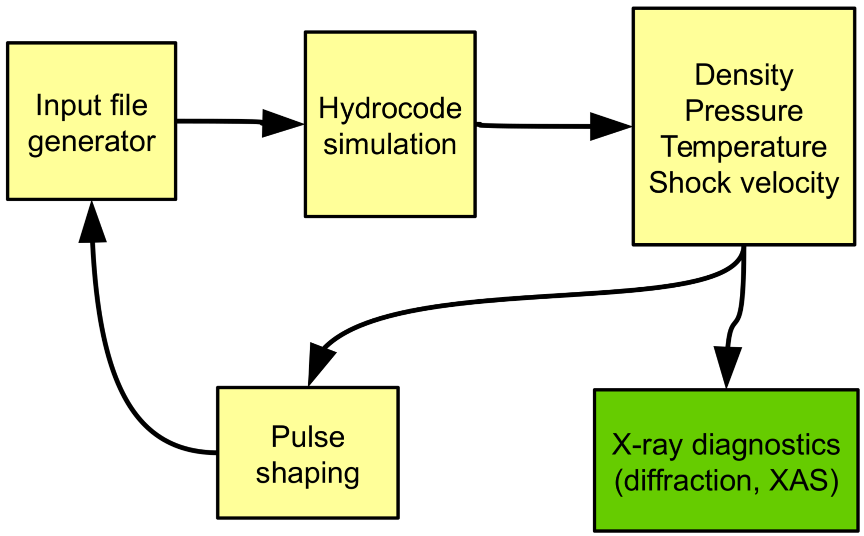
# Baseline science application #3: WDM

## X-ray probing shock compressed warm dense matter (WDM)

- Model high energy, long pulse (ns) laser driven shock compression with 1D & 2D radiation hydrodynamic codes
- Simulate XAFS (& scattering) signals
- Pulse optimization via feedback of simulated signal to pulse shaper

Torchio et al. Scientific Reports (2016)

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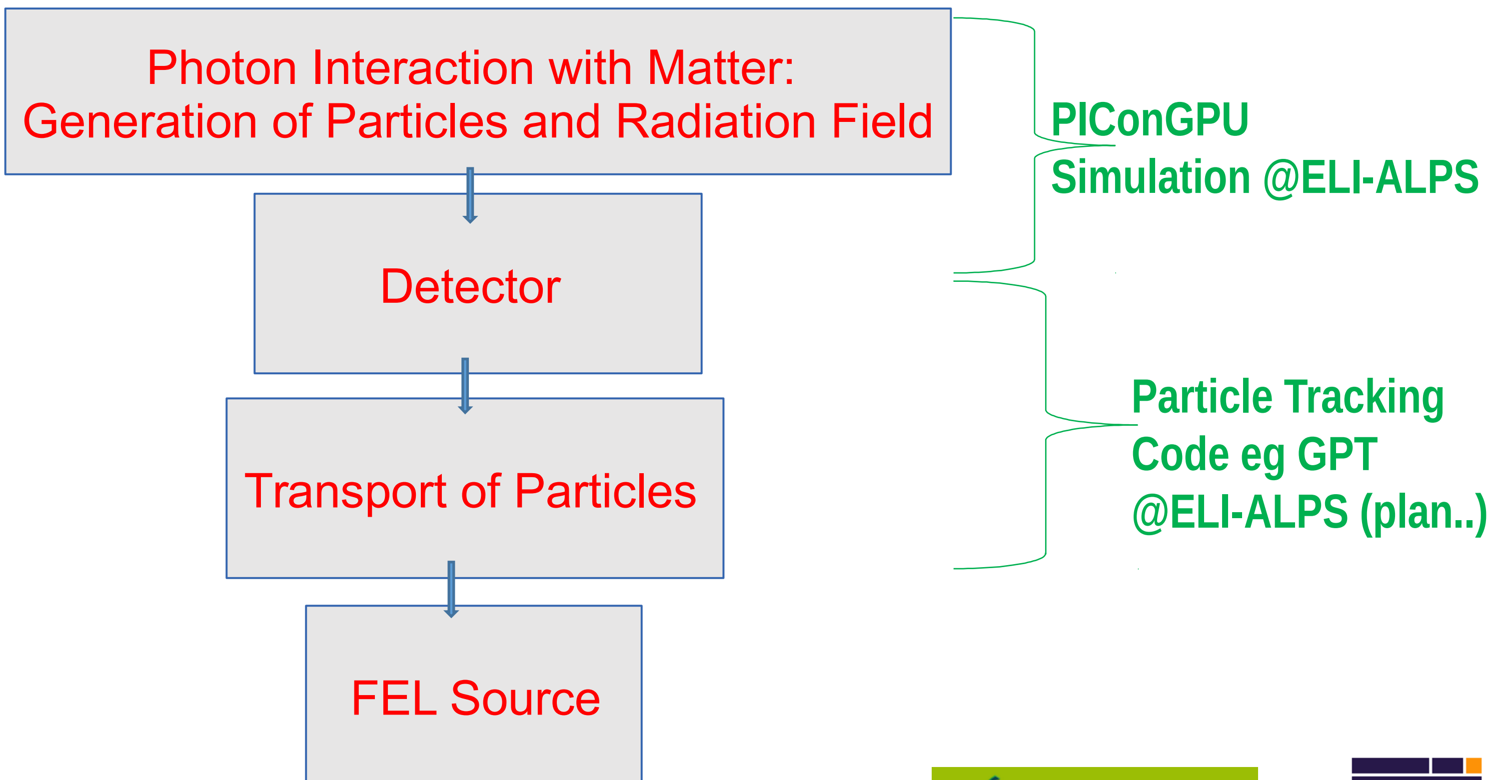
# Science application #4

## Laser-plasma acceleration based x-ray source

- Model laser wakefield acceleration (PIC)
- Feed electrons into FEL simulation code

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# Simulation Data Interfaces

| | Source | Propagation | PMI | Scattering | Detector | Lead institute |
|---|---|---|---|---|---|---|
| **SPI** | FAST | WPG/SRW | XMDYN & XATOM | singFEL | X-CSIT | EU.XFEL |
| **HPL** | FAST | WPG/SRW | PIConGPU | paraTAXIS | X-CSIT | HZDR |
| **WDM** | Oasys | | Esther (1D-Rad-Hydro) | XRTS / FEFF | | ESRF |

- Standardized hdf5 file structure
- Subsequent *Calculators* check mutual dataset consistency

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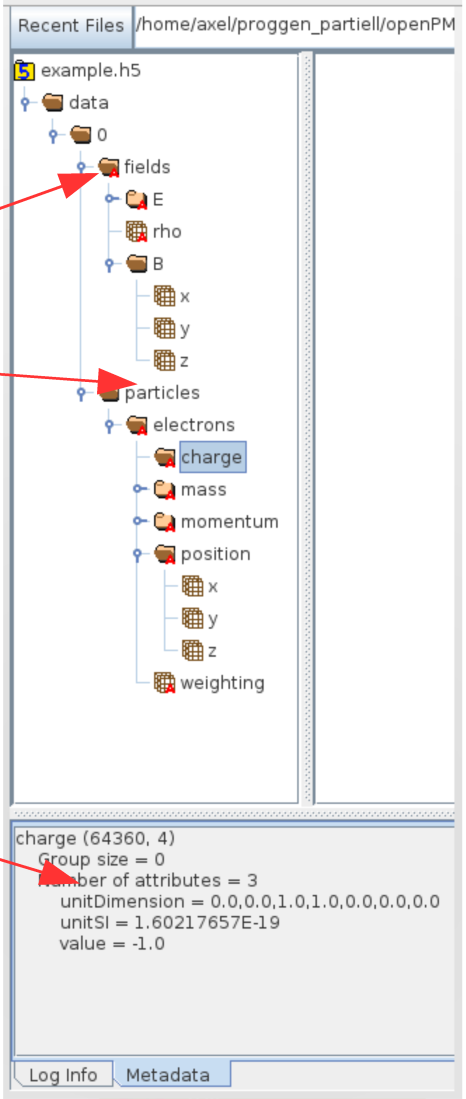
# openPMD: An open standard for particle-mesh data 🕮 http://www.openpmd.org

- Standardized hierarchical organization of (meta)data for fields and particles

- Independent of file format:
  - hdf5 serial
  - hdf5 parallel
  - adios

- Supports all unit systems through standardized unit conversion scheme

- Application specific domain extensions:
  - PIC
  - Rad-Hydro (in progress)

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# Single Particle Imaging simulations with SIMEX

**Single Particle Imaging (SPI) at X-FELs may provide structure data at Angstrom resolution. Among open questions, the most pressing are:**

- Understand role of radiation damage processes
- Study effect of XFEL pulse properties

**Simulations can provide guidelines through systematic parameter scans**

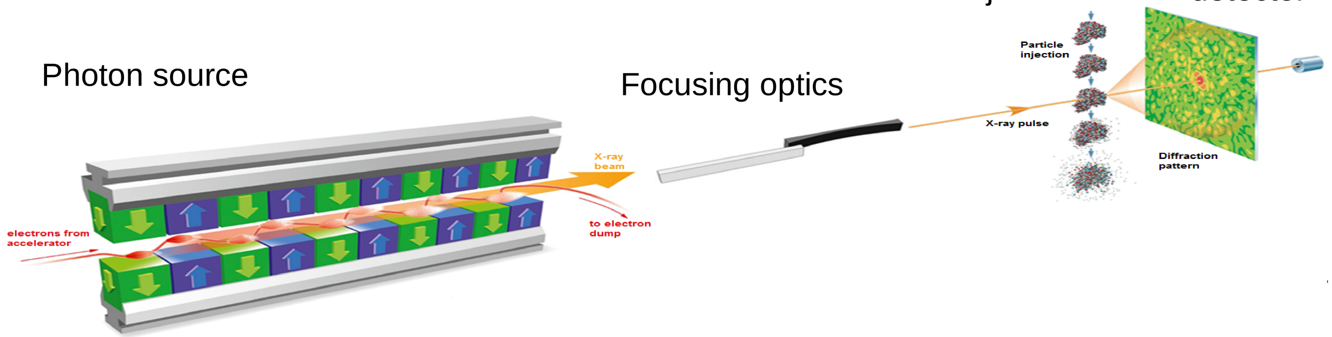
Baseline setup

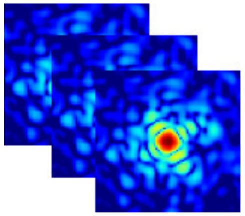
Photon source

Focusing optics

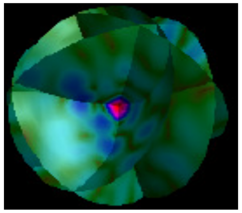
Sample injection

Pixel area detector

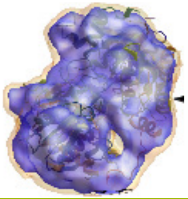


Orient



Phase



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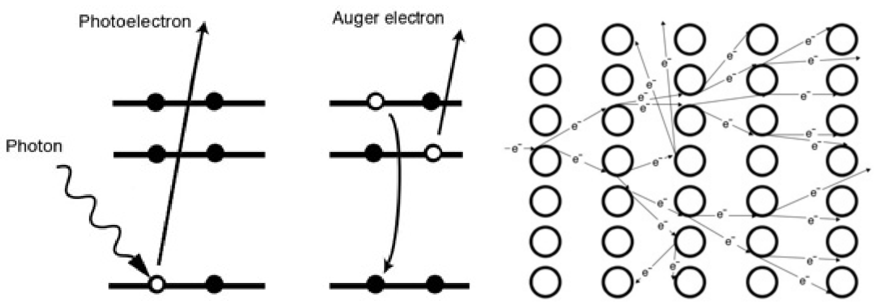
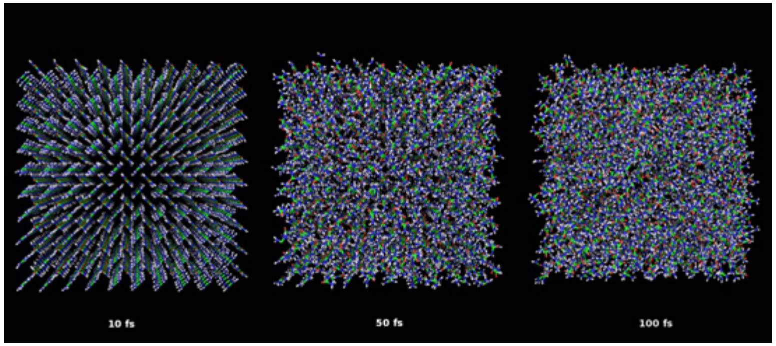
# Radiation damage processes and timescales

- SPI paradigm: Use ultrashort, intense x-ray pulses to diffract from single particles
→ Scatter enough photons despite small scattering cross-section and few scatterers
→ Probe before destruction

Neutze et al. Nature (2000)

desy.cfel.de/cid/research/understanding_the_physics_of_intense_x_ray_interactions/




0 1 10 100 fs

| Atom | $\tau_{Auger}$(fs) |
|---|---|
| C | 10.7 |
| N | 7.1 |
| O | 4.9 |
| S | ~ 2 fs |
| P | ~ 2 fs |

- Ultrashort pulses (few fs) may outrun <u>secondary ionization</u> and <u>hydrodynamic expansion</u>
- ↔ Short pulses contain less photon

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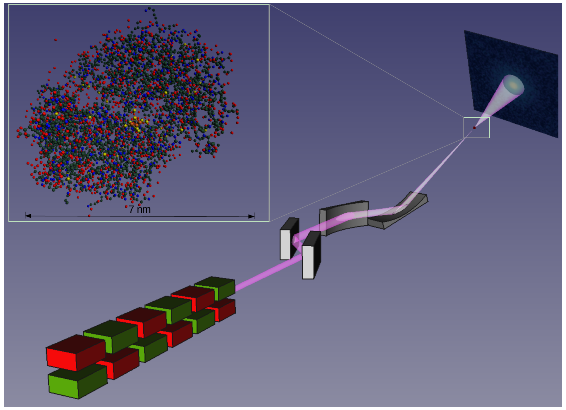
# Simulation parameters

## FEL

- Pulselength 3fs, 9 fs, 30 fs
- Photon energy 4.96 keV
- FEL saturation nz = 35m

## Sample

- Two-nitrogenase protein (2NIP)
- ~5000 non-H atoms Schlessman et al. J. Mol. Biology (1998)
- Iron-Sulfur ligand “SF4“
- Known crystallographic structure (PDB)




## Detector

- 80 x 80 superpixels of 1200 µm size
  13 cm sample-detector distance
  max resolution = 3.5 Å (edge)
- Poissonization of incoming intensity
- Particle, charge, electronics simulation omitted here

## Simulation

- ~40 pulses from FAST XFEL Pulse Database
- Propagation: WPG (SPB-SFX beamline)
- PMI: ~1000 Sample trajectories 100 snapshots per trajectory
- Apply random rotation of atom coordinates to each trajectory
- 200 diffraction patterns per trajectory

  → 200000 patterns

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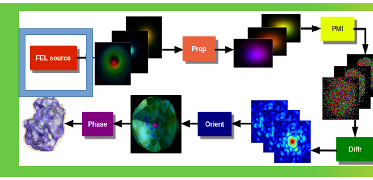
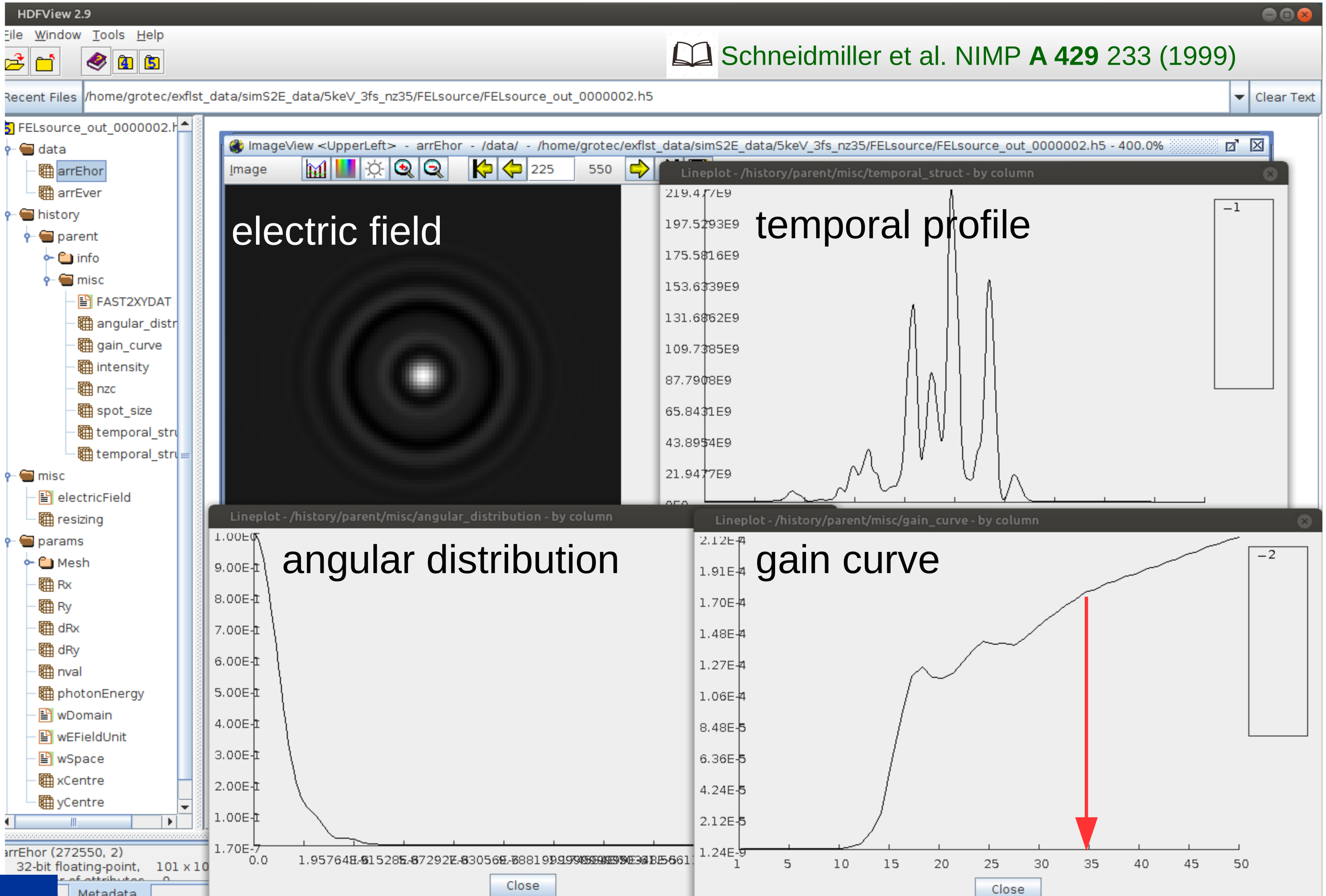
X F E L pulses simulated with FAST code

# Pulse database at https://in.xfel.eu/xpd

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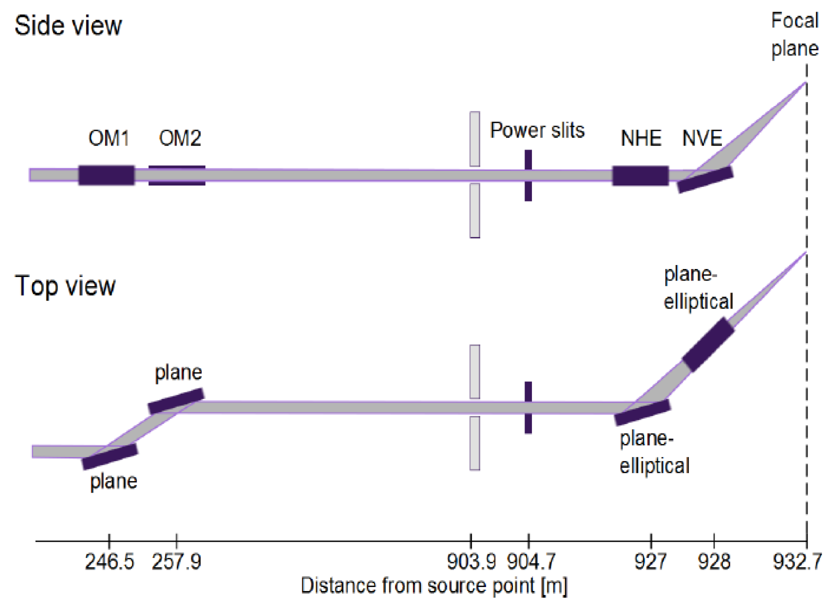
# Wave propagation (WPG library)

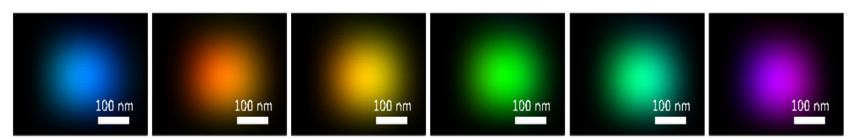
**S**ynchrotron **R**adiation **W**orkshop

- C library for  wavefront propagation (coherent sources)

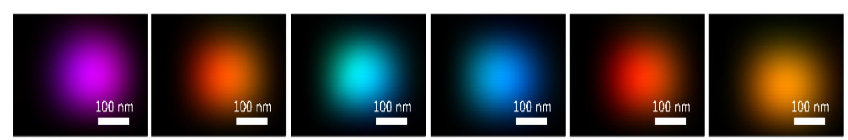
**W**ave **P**ropa**G**ator

- Python frontend for SRW




color: phase brightness: intensity $\Delta t=0.2$ fs





📖 Samoylova et al. J. Appl. Cryst. (2016)
📖 Chubar et al. NIMP **A593**, 30 (2008)
📖 Yoon et al. Scientific Reports **6** 24791 (2016)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# Photon-Matter interaction: Molecular Dynamics + Ab-initio electronic structure

Jurek et al. J. Appl. Cryst. (2016)

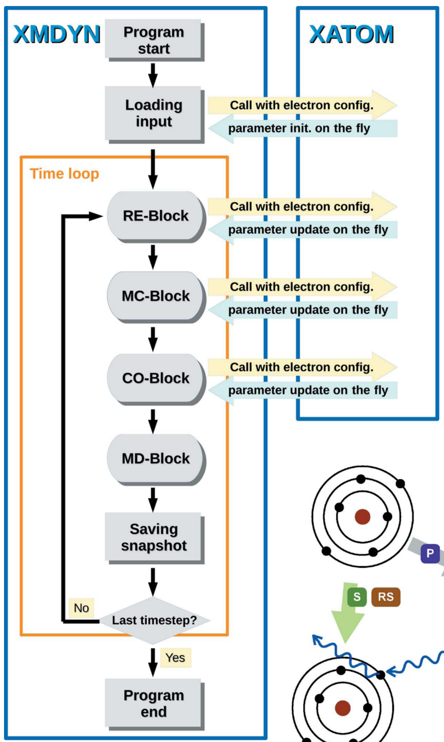
Son et al. Phys. Rev. A **83**, 033402 (2011)

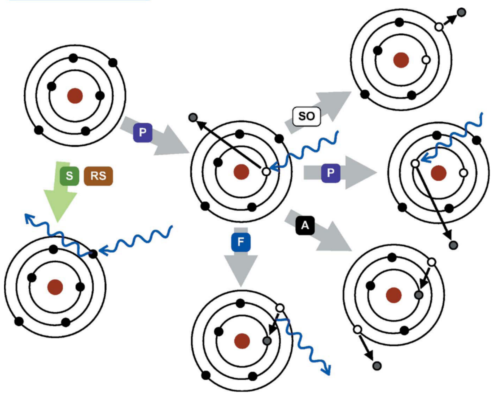
## XMDYN & XATOM

- Ions move according to Newtonian mechanics
- MonteCarlo simulates electronic transitions according to rates/cross-sections from
- Ab-initio (Hartree-Fock-Slater) electonic structure code (XATOM)
- Output:
  - Atom positions $\mathbf{R}_i(\mathbf{r},t)$
  - Electronic structure $\{n_a\}_i(t)$

    → form factors $f(\mathbf{k},t)$

    structure factors $S(\mathbf{k}, t)$

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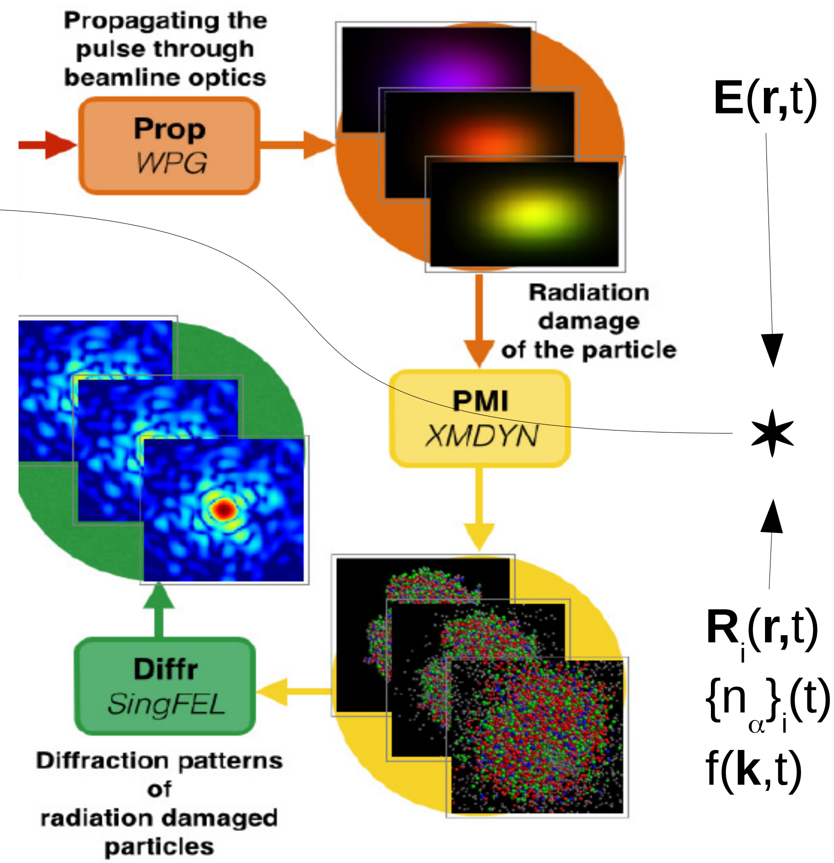
# singFEL propagates photons scattered from the sample to the detector plane

## Diffraction from single particles

$$I_c(q/2,\Omega) = \Omega \frac{d\sigma_T(\theta)}{d\Omega}\int_{-\infty}^{\infty} I_i(t)\left(\boxed{|F_c(q/2,t)|^2}+\boxed{S_c(q/2,t)}+\boxed{N_c^{free}(t)}\right)dt$$

- Coherent scattering from bound electrons
- Incoherent (Compton) scattering from bound electrons
- Compton scattering from free electrons




Yoon et al. Scientific Reports **6** 24791 (2016)

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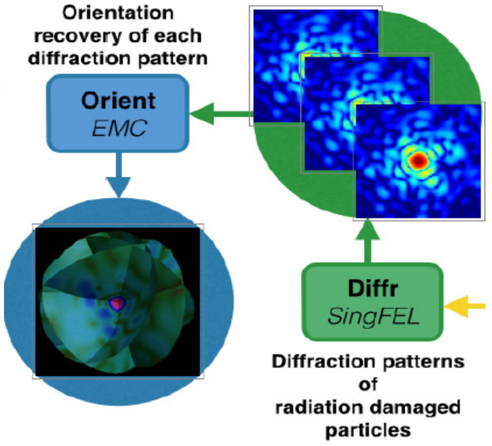
# Electron density reconstruction from simulated diffraction patterns

**Orientation of 2D diffraction patterns into a 3D diffraction volume**

- **E**xpand-**M**aximize-**C**ompress algorithm

$$W_{i+1}(\mathbf{p}) = \mathrm{C} \cdot \mathrm{M} \cdot \mathrm{E} \cdot W_i(\mathbf{p})$$

Yoon et al. Scientific Reports **6** 24791 (2016)

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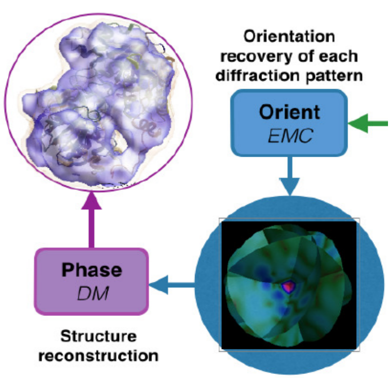
# Electron density reconstruction from simulated diffraction patterns

## Phase retrieval for electron density reconstruction

- **D**ifference **M**ap algorithm
  - Problem: Intensity ~ |**E** exp(i$\phi$) |$^2$
  - Constrained through finite support and positivity of electron density.
  - Iteratively minimize difference between support projection and Fourier projection.

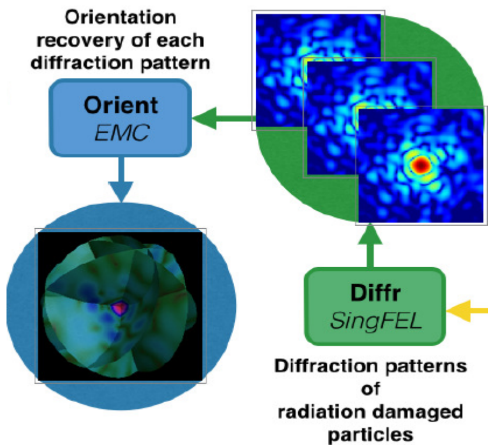



## Orientation of 2D diffraction patterns into a 3D diffraction volume

- **E**xpand-**M**aximize-**C**ompress algorithm

$$W_{i+1}(\mathbf{p}) = \mathrm{C} \cdot \mathrm{M} \cdot \mathrm{E} \cdot W_i(\mathbf{p})$$

Yoon et al. Scientific Reports **6** 24791 (2016)

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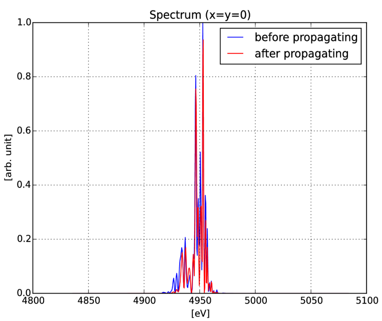
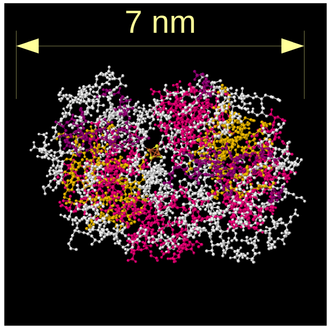
# SIMEX simulations put lower limit on XFEL pulse length for single particle imaging applications





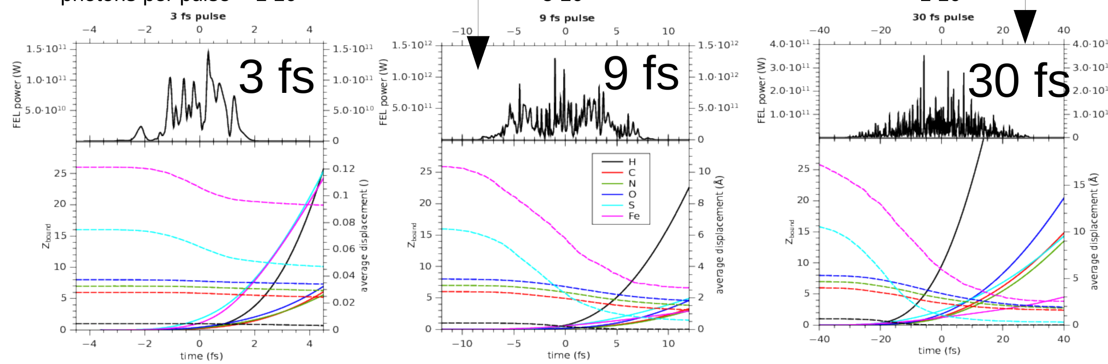

pulse spectrum before and after propagation



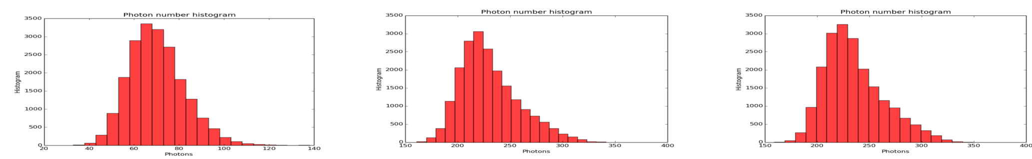

sample molecule 2NIP

Yoon et al. Sc. Rep. (2016)

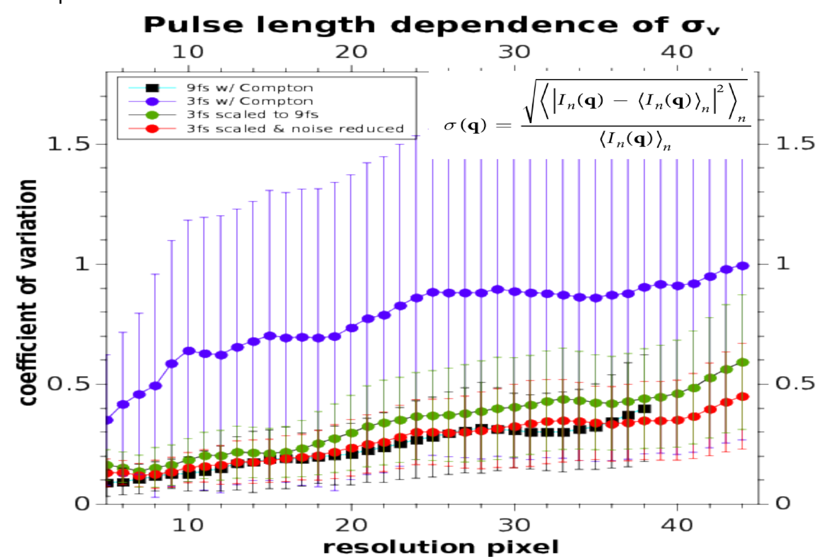
photons per pulse = $1 \cdot 10^{11}$ $5 \cdot 10^{11}$ $1 \cdot 10^{12}$




Bound electrons and avg. displacement during irradiation




diffracted photons = 70+/-12 230+/-28 234+/-29

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DESY — M. Yurkov, E. Schneidmiller

CFEL SCIENCE — Z. Jurek, B. Ziaja, R. Santra

SLAC — C.H. Yoon

NUS National University of Singapore — N.D. Loh

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# Summary and Conclusions

- **simex_platform** is a rapidly growing modern software suite for photon science experiment simulations.
- Generic user interfaces facilitate usage of advanced simulation software.
- Open standards for data exchange between simulation codes enable new applications and integration of 3rd party codes.
- 1st science application demonstrates the usefulness, applicability, and validity of **simex_platform.**

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# Acknowledgements

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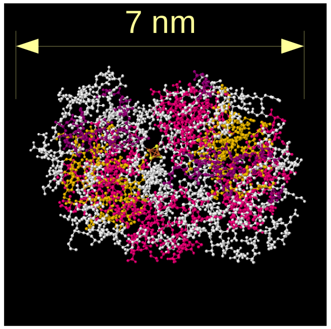
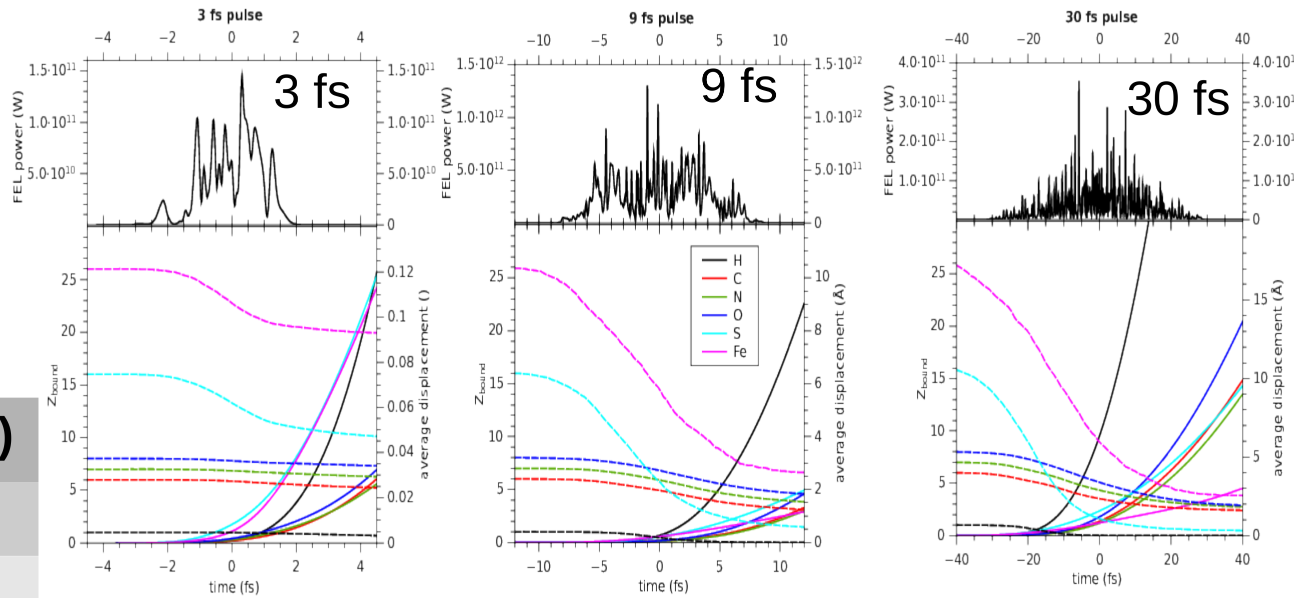
# Photon matter interaction and diffraction



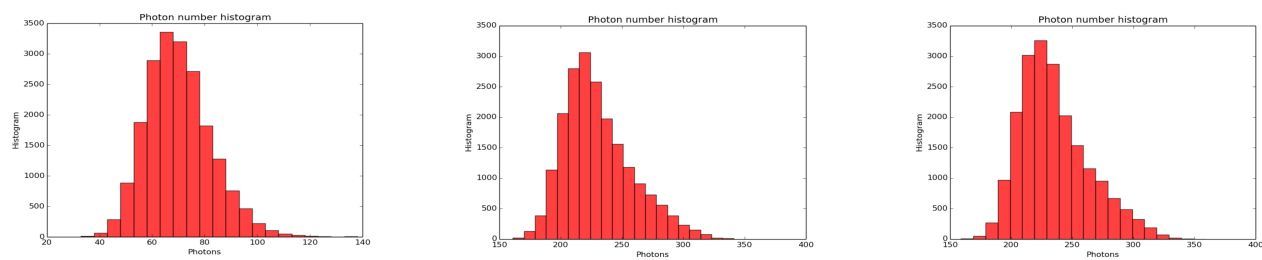

sample molecule 2NIP

| Atom | $\tau_{Auger}$(fs) |
|---|---|
| C | 10.7 |
| N | 7.1 |
| O | 4.9 |
| S | ~ 2 fs |
| Fe | ~ 2 fs |

photons per pulse = $1 \cdot 10^{11}$ $5 \cdot 10^{11}$ $1 \cdot 10^{12}$




Bound electrons and avg. displacement during irradiation




diffracted photons = 70+/-12 230+/-28 234+/-29

📖 CFG et al., in preparation 📖 Yoon et al. Scientific Reports **6** 24791 (2016)

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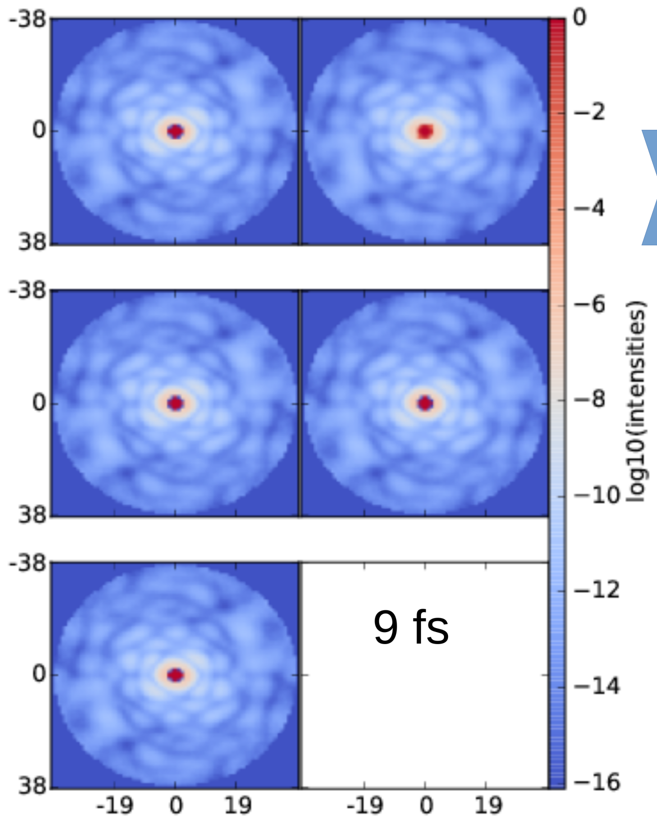
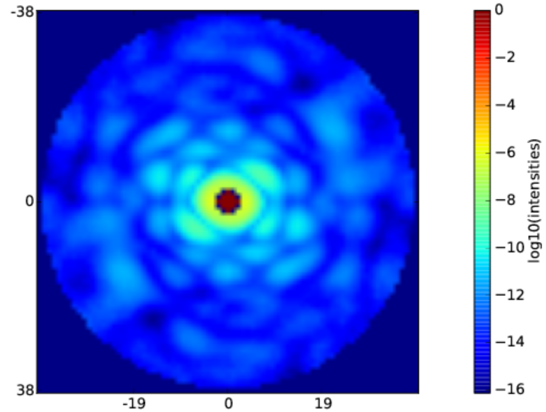
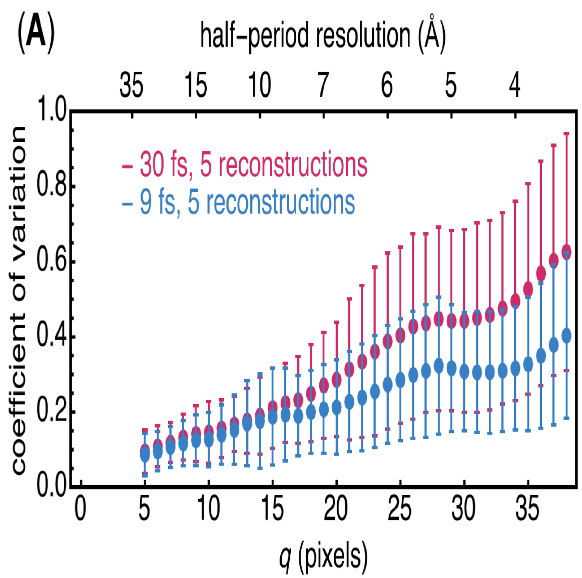
# Quantifying 3D diffraction volume consistency: The coefficient of variation

Each run starts from a new, random initialization




$$\sigma(\mathbf{q}) = \frac{\sqrt{\left\langle \left| I_n(\mathbf{q}) - \langle I_n(\mathbf{q}) \rangle_n \right|^2 \right\rangle_n}}{\langle I_n(\mathbf{q}) \rangle_n}$$

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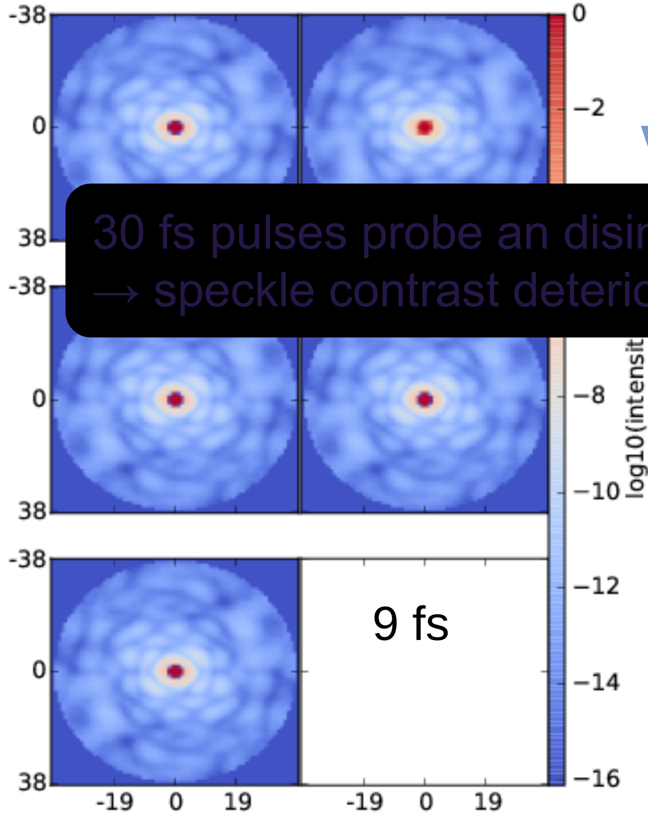


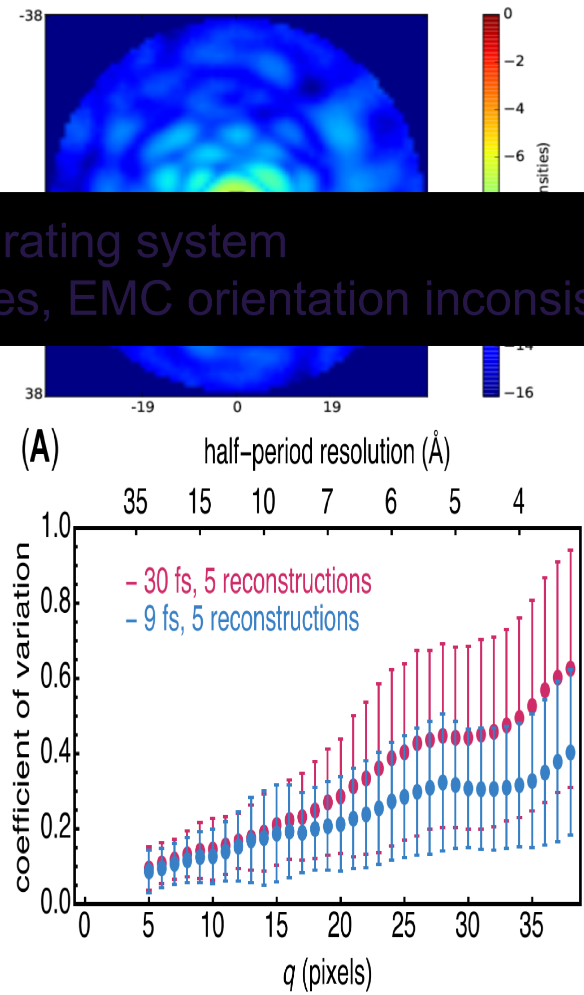


$$\sigma(\mathbf{q}) = \frac{\sqrt{\left\langle \left| I_n(\mathbf{q}) - \langle I_n(\mathbf{q})\rangle_n \right|^2 \right\rangle_n}}{\langle I_n(\mathbf{q})\rangle_n}$$

30 fs pulses probe an disintegrating system
→ speckle contrast deteriorates, EMC orientation inconsistent

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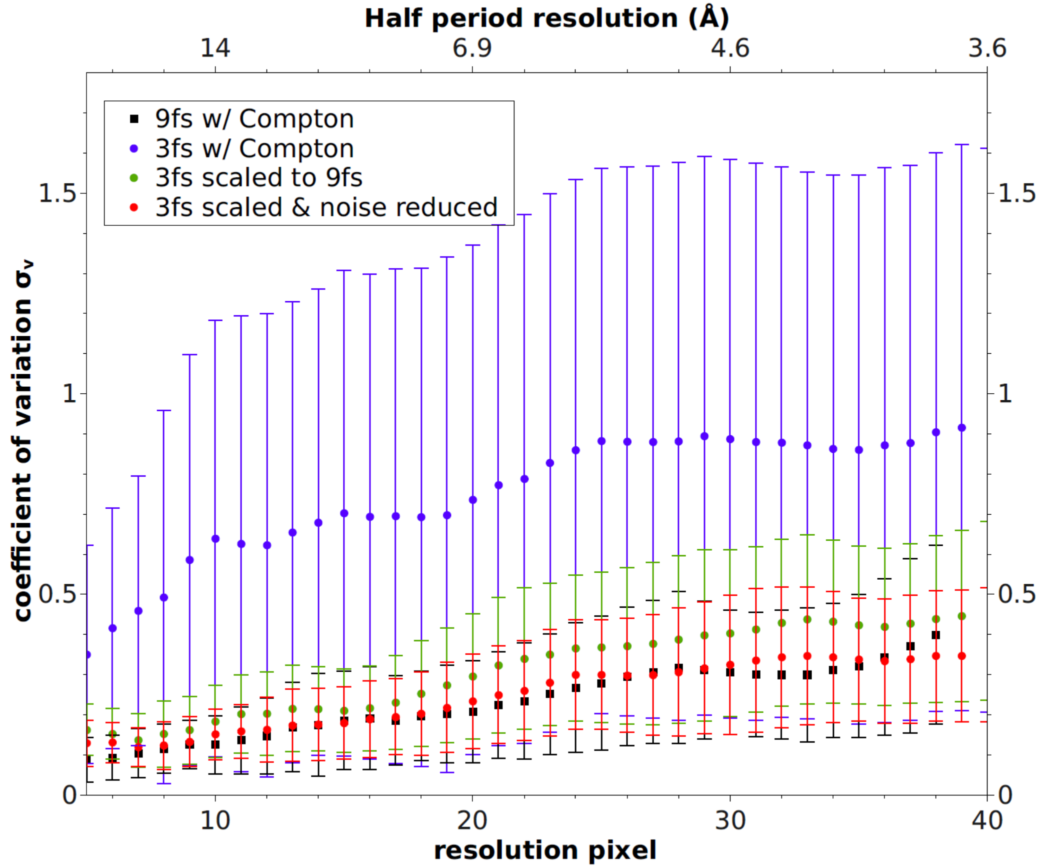
# Oriented 3 fs diffraction patterns show 2-3 times larger variation than 9 fs data



$$\sigma(\mathbf{q}) = \frac{\sqrt{\left\langle \left| I_n(\mathbf{q}) - \langle I_n(\mathbf{q}) \rangle_n \right|^2 \right\rangle_n}}{\langle I_n(\mathbf{q}) \rangle_n}$$




3 fs diffraction data suffers from low photon count and S/N, prohibitive for EMC to give consistent orientations despite low ionization and absence of ionic displacement

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