EUCALL

SIMulation of EXperiments

Carsten Fortmann-Grote

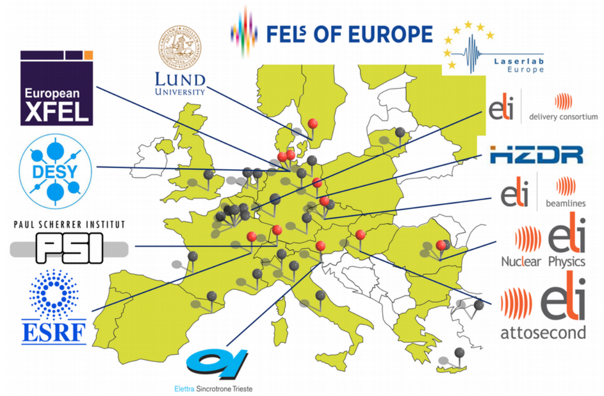
This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 654220

Software for Optical Simulations WORKSHOP Trieste, 3rd – 7th October 2016

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

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

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

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

SIMEX personnel

European XFEL: A. P. Mancuso, C. Fortmann-Grote

HZDR (Helmholtz Zentrum Dresden Rossendorf): M. Bussmann, A. Huebl, A. Grund, M. Garten

ESRF: S. Pascarelli, R. Torchio, R. Briggs

DESY: F. Schlünzen, S. Yakubov

ELI attosecond: A. Andreev, A. Sharma, M. Sedov, S. Kalmykov

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

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

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

SIMEX' objective

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

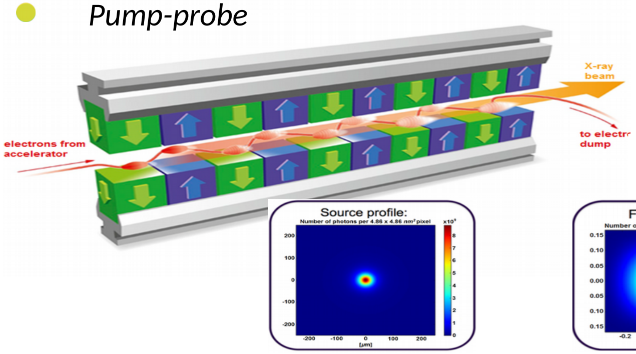
Target/Sample
- *Atoms, molecules, clusters*
- *Solids, surfaces*
- *Liquids*
- *Plasmas*

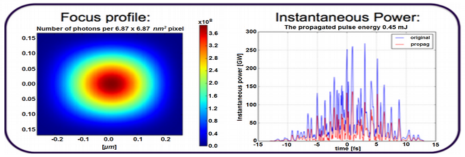
Photon Data Analysis
- *Structure determination*
- *Electronic structure*
- *Transport*
- *Relaxation & Thermodynamics*

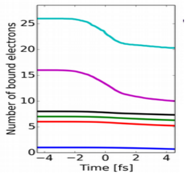
Diagnostics
- *Spectroscopy*
- *Diffraction*
- *Scattering*

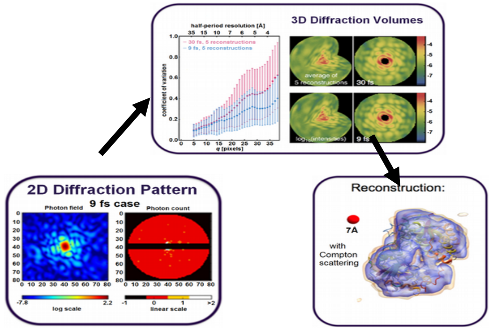
Photon propagation
- *Lenses*
- *Mirrors*
- *Apertures, slits*

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









SPI simulation framework: simS2E
→ Yoon et al. Science Rep. (2016)

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

Some highlights about simex_platform

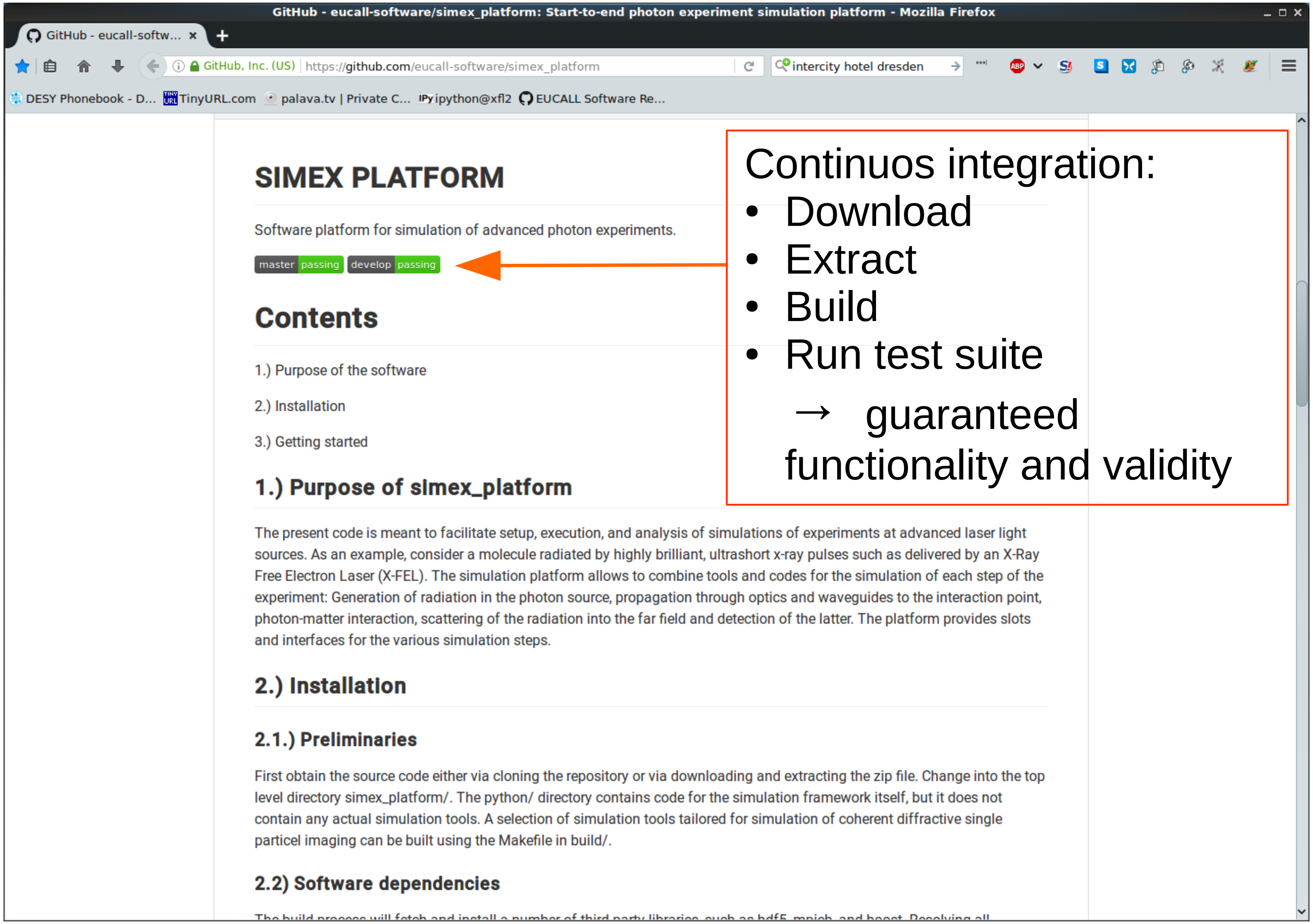
- Modular simulation platform for source-to-detector simulations in photon science
- Opensource (www.github.com/eucall-software/)
- Interfaces for various photon-matter interaction codes ready
- Various deployment options: Makefile, binaries, and Docker containers
- Performance boosts for 3rd party simulation codes up to 160x

→Poster by S. Yakubov

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

EUCALL

SIMEX platform is on github


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

https://github.com/eucall-software/simex_platform

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

The build process will fetch and install a number of third party libraries, such as hdf5, mpich, and boost. Resolving all

Continuos integration:

- Download
- Extract
- Build
- Run test suite

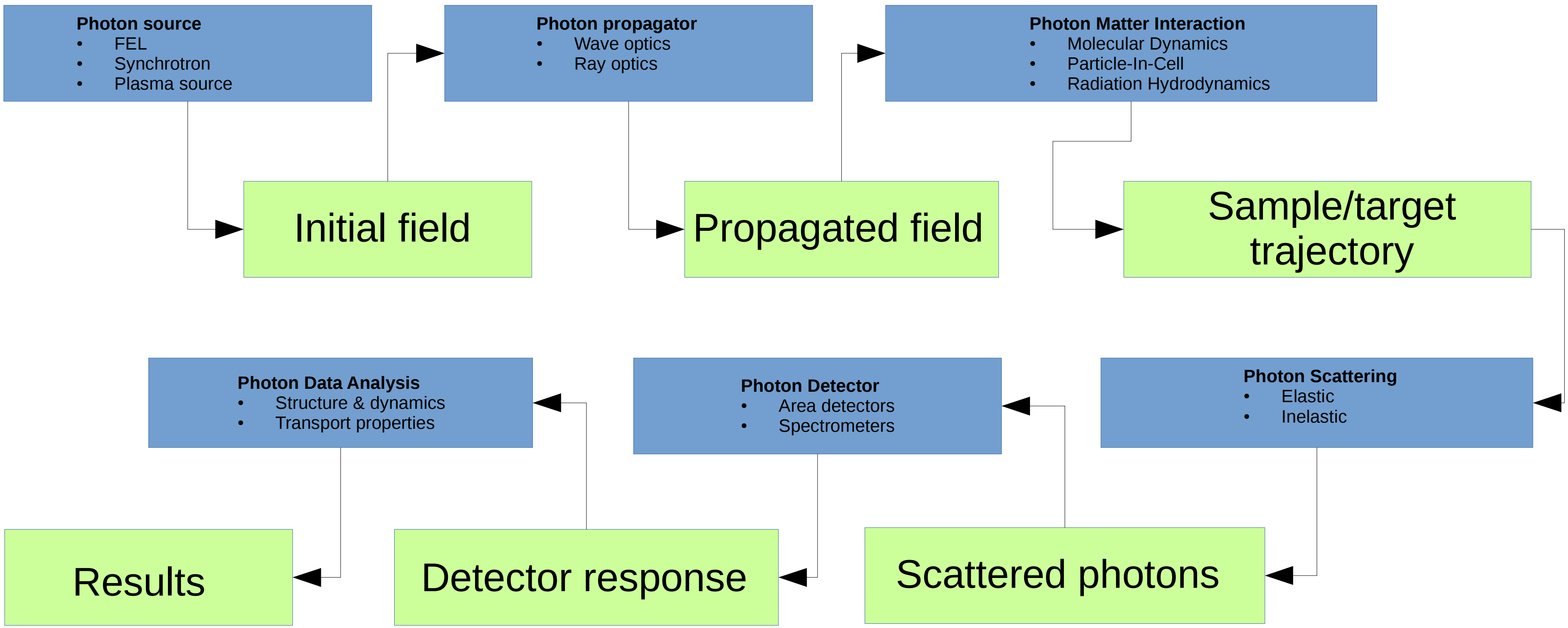
→ guaranteed functionality and validity

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

Calculators and Interfaces in simex_platform

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

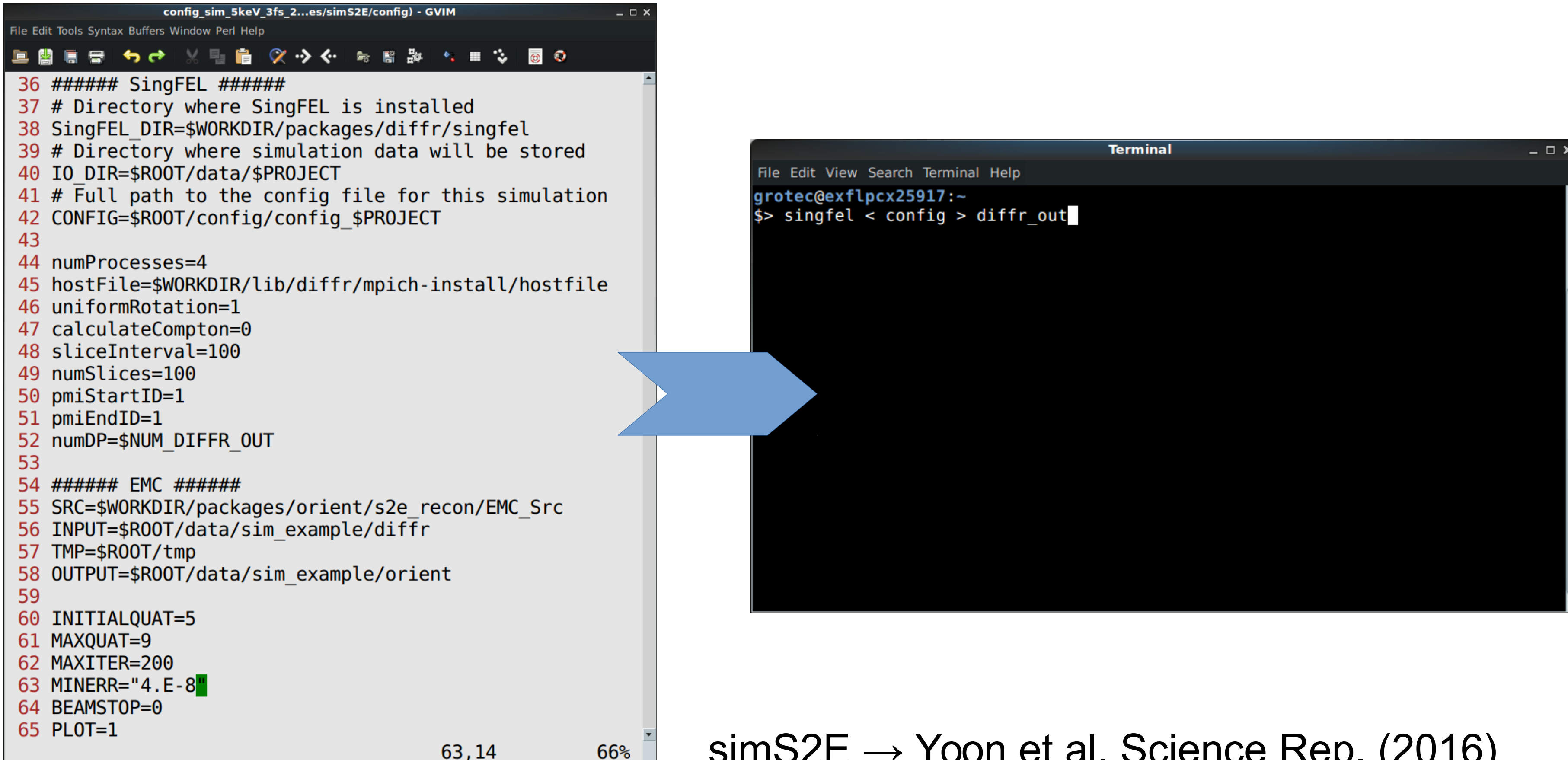
Interfaces: hdf5 file + format description (simS2E, openPMD)



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

European XFEL

User interface: from input decks ...



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

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

… to Calculators

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

File Edit Tools Syntax Buffers Window Perl Help

W/X/S/r/3fs_emc.py W/X/C/s/c/config_sim_5keV_3fs_2NIP

```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_parameter
s)

# 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.
                                                    41,1          Bot
```

Terminal

File Edit View Search Terminal Help

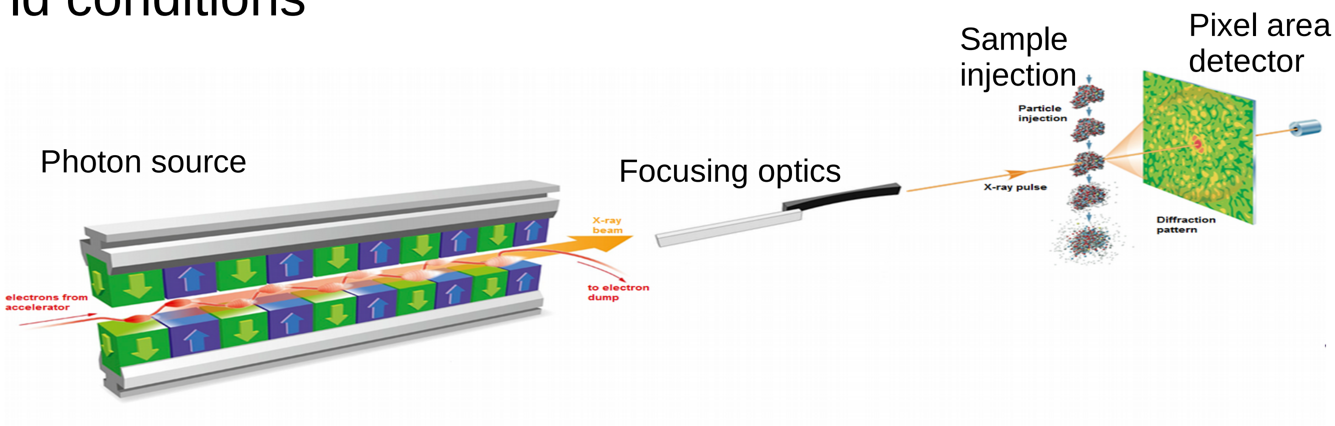
```
grotec@exflpcx25917:~
$> python diffr_emc.py
```

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

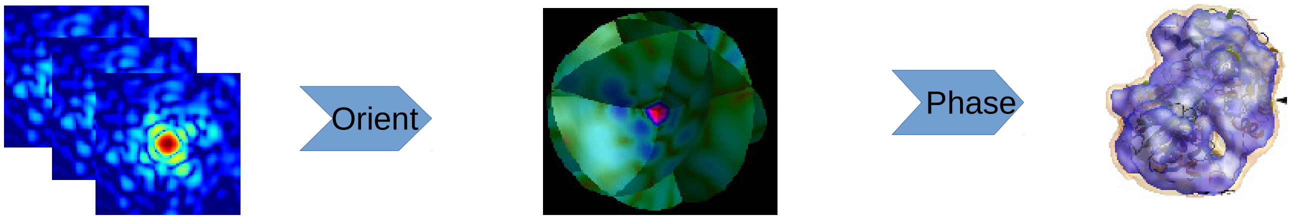
Baseline science application #1: SPI

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



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

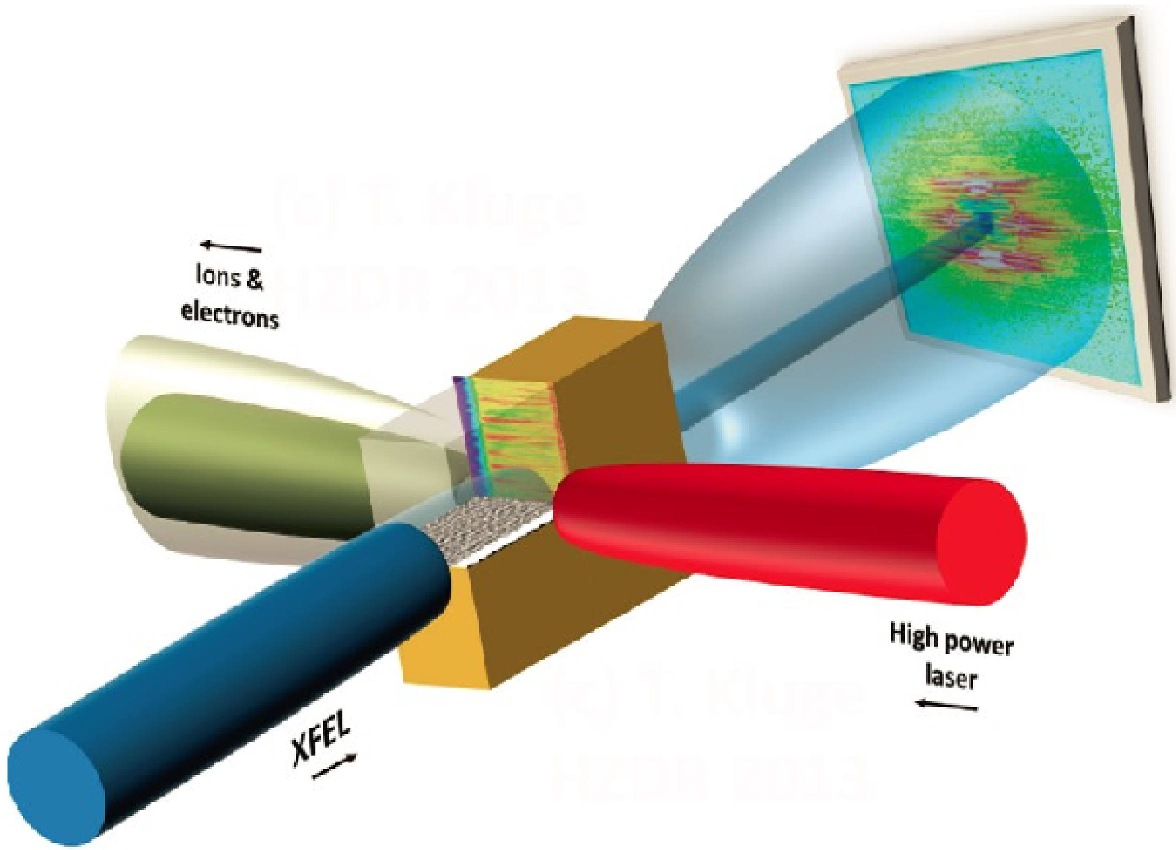
Baseline science application #2: HPL

X-ra

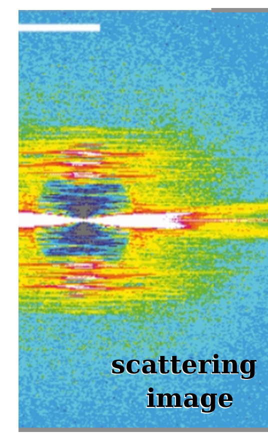
Example Setup for Probing of Ultrafast Laser-Matter Interaction

- M
  p
- C
- E

ited



XFEL beamli



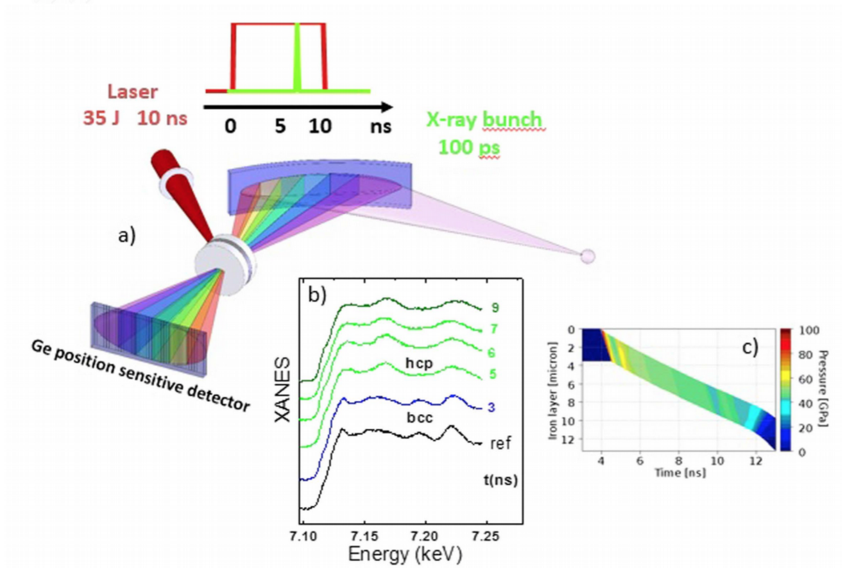
This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 654220

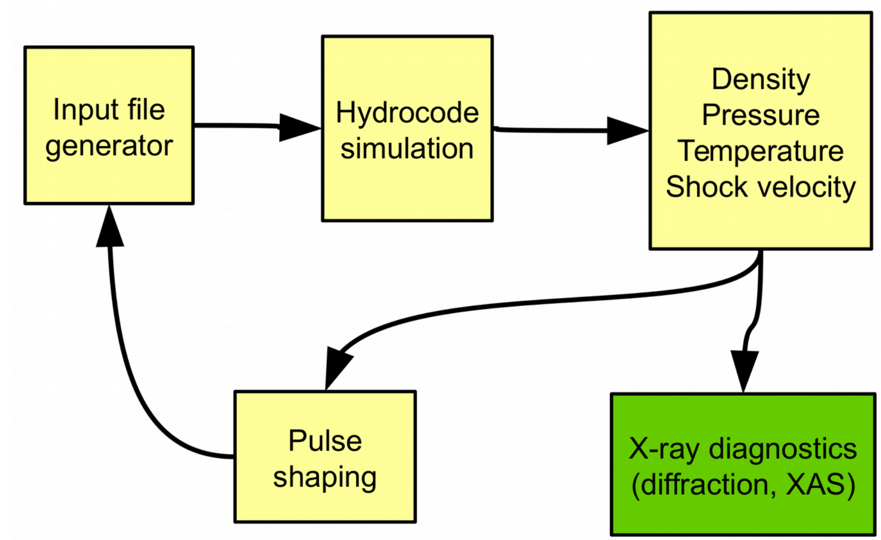
Baseline science application #3: WDM

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)

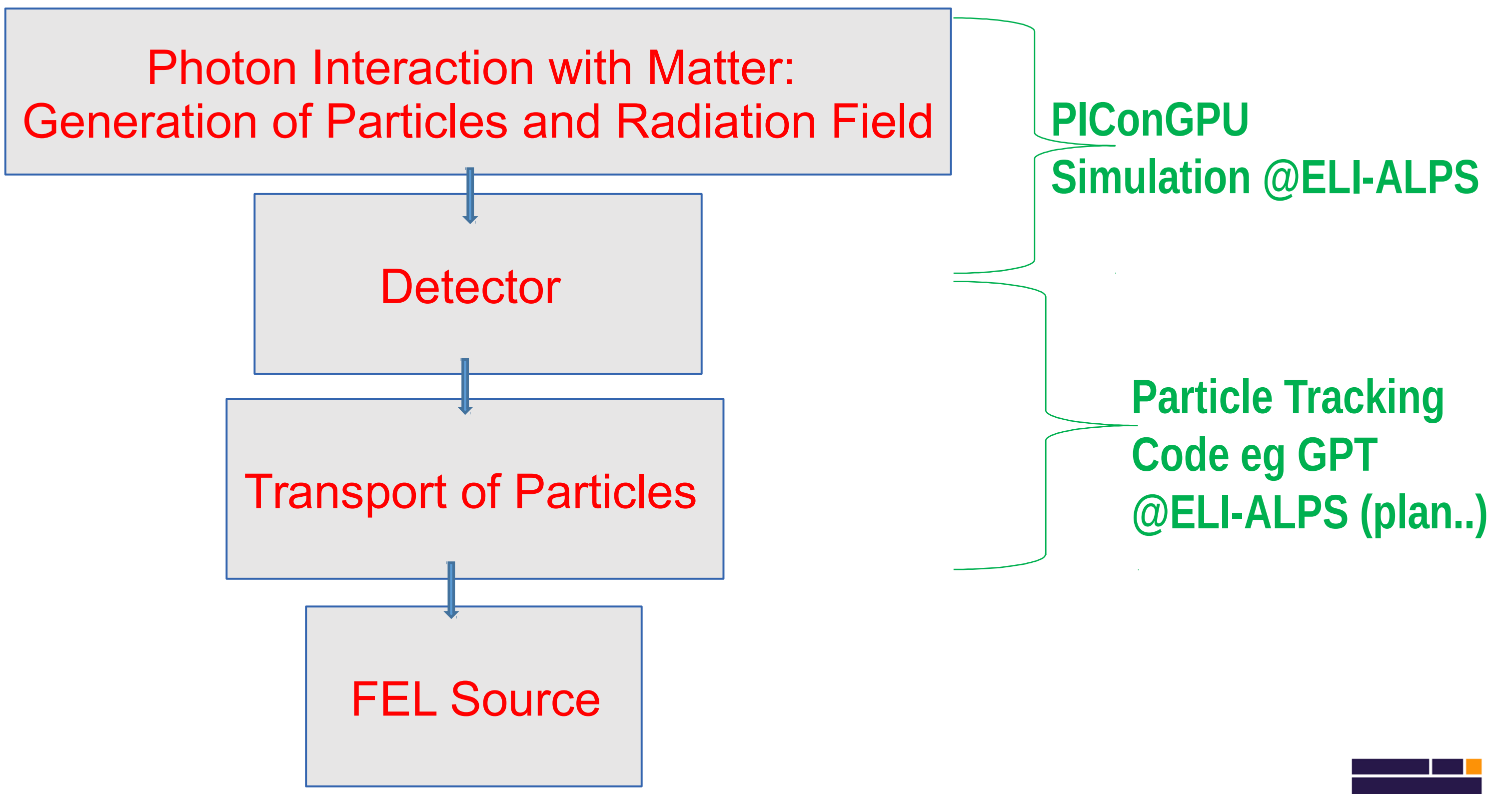




This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 654220

Laser-plasma acceleration based x-ray source

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



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

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			Esther (1D-Rad-Hydro)	XRTS / FEFF		ESRF

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

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

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

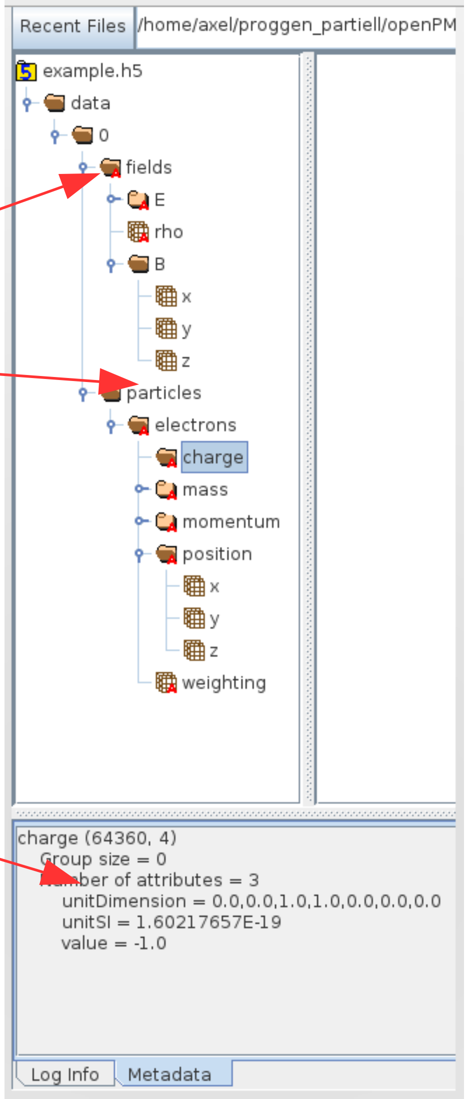
- Standardized hdf5 file structure
- Subsequent *Calculators* check mutual dataset consistency

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

The openPMD standard for particle-mesh data

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 <u>all</u> unit systems through standardized unit conversion scheme
- Application specific domain extensions:
  - PIC
  - Rad-Hydro (in progress)



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

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:

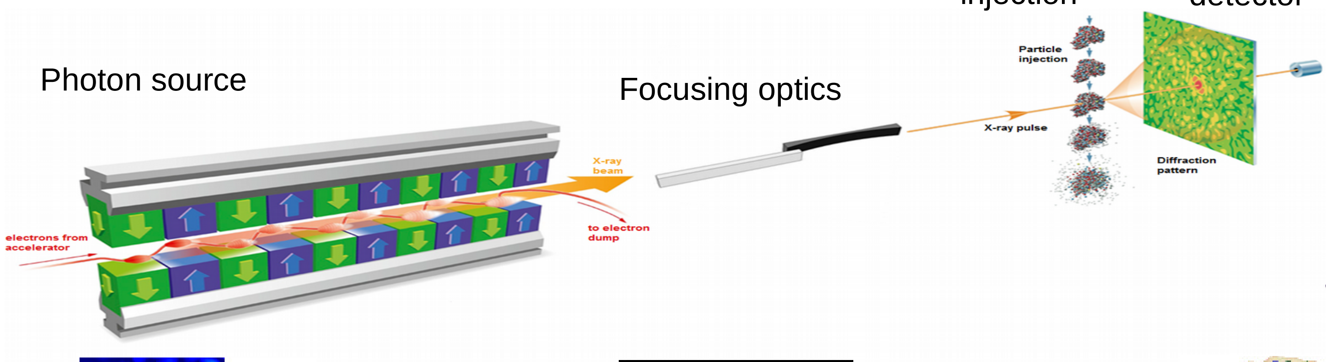
- Understand role of radiation damage processes
- Study effect of XFEL pulse properties

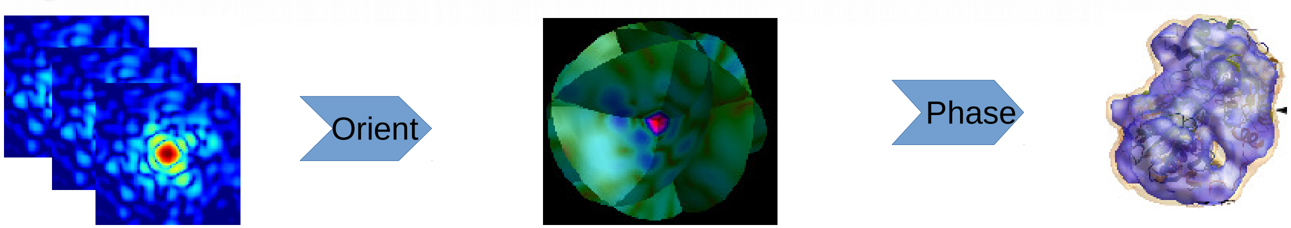
Simulations can provide guidelines through systematic parameter scans

Sample injection

Pixel area detector

Baseline setup



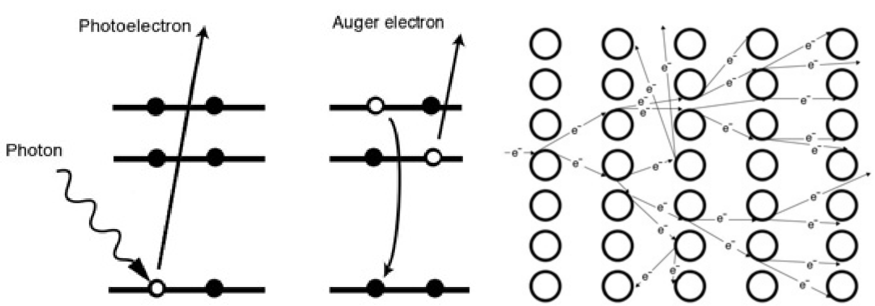


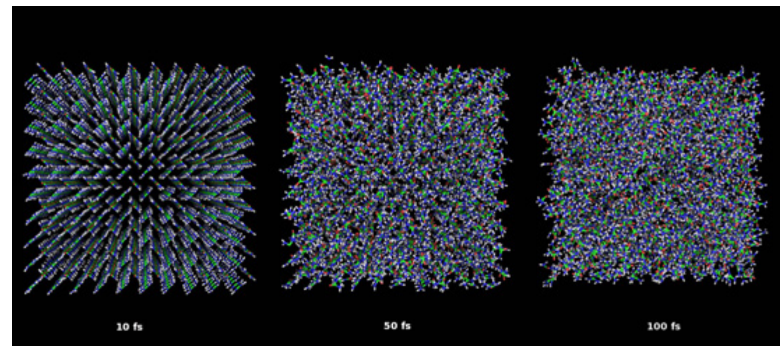
This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 654220

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	τ_{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

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

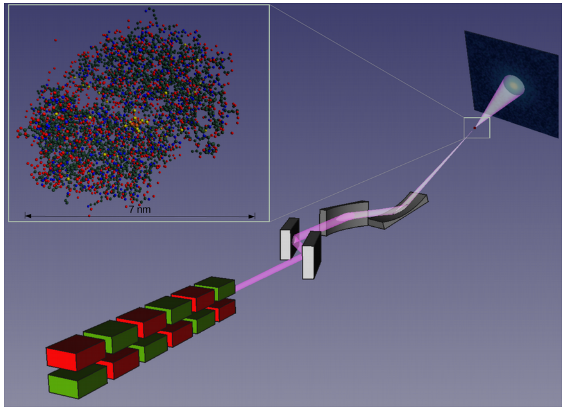
Simulation parameters

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

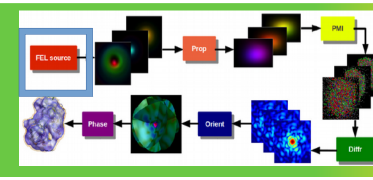
Simulation

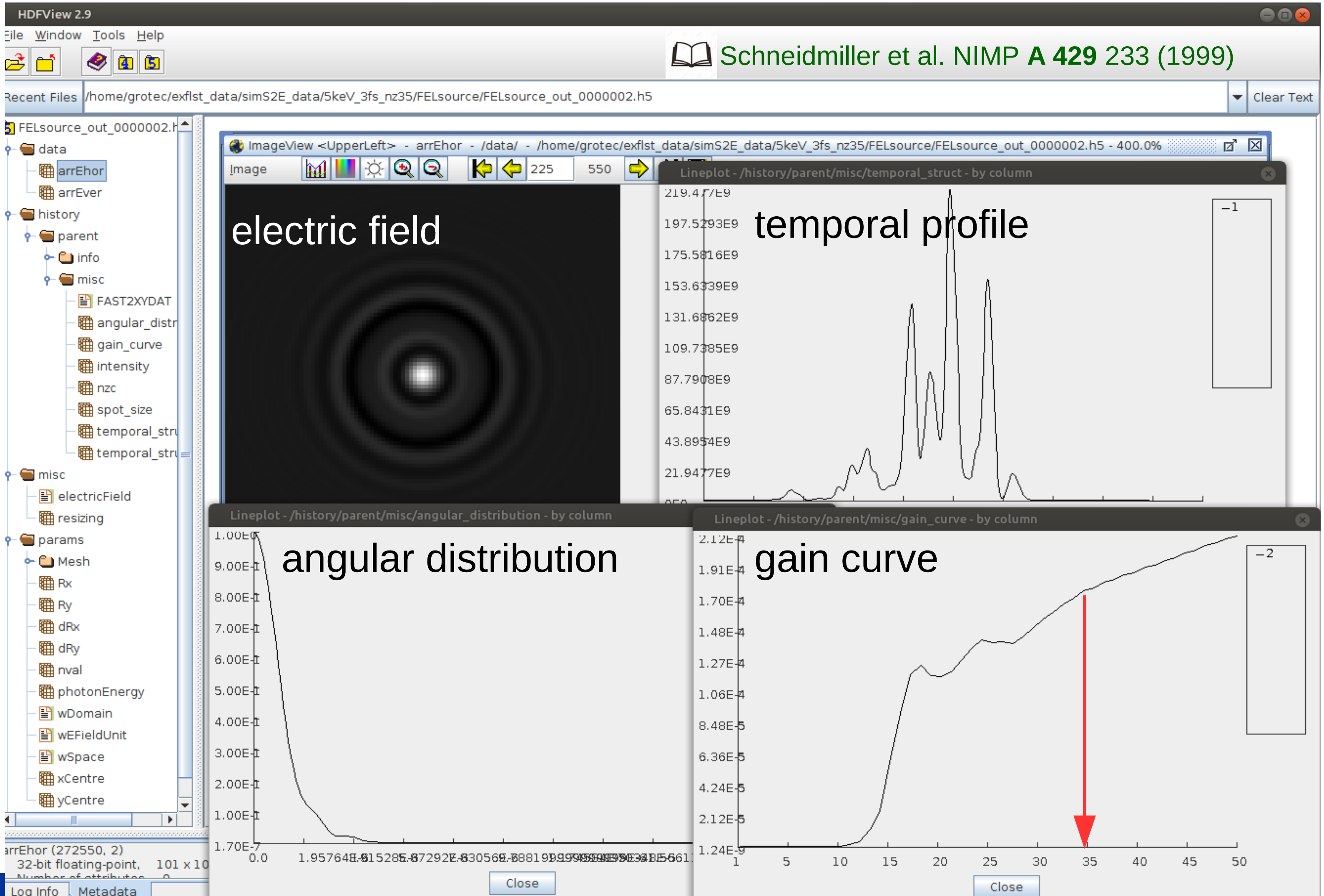
- ~40 pulses from FAST XFEL Pulse Database
- Propagation: WPG (SPB-SFX beamline)
- PMI: ~1000 Sample trajectories 100 snapshots per trajectory
- Apply random rotation of atom coordinates to each trajectory
- 200 diffraction patterns per trajectory

  → 200000 patterns

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

XFEL pulses simulated with FAST code
Pulse database at https://in.xfel.eu/xpd





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

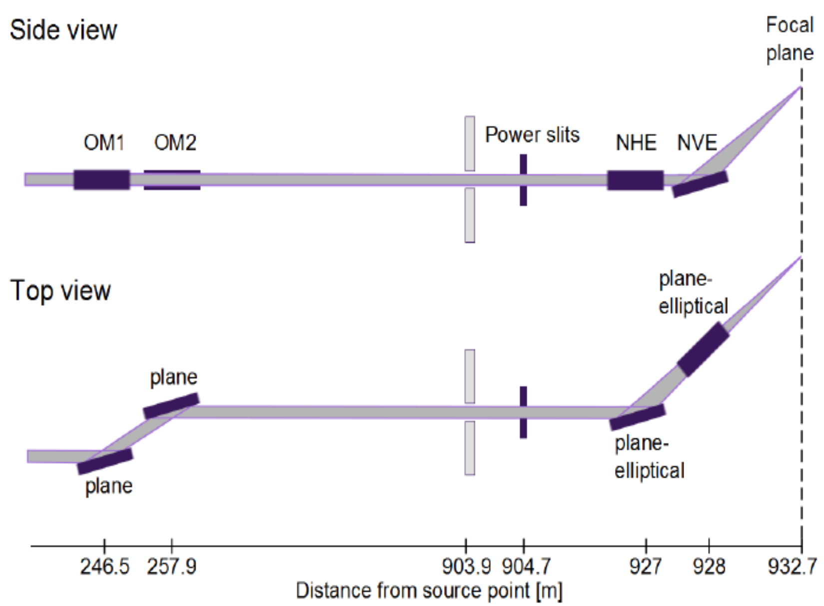
Wave propagation (WPG library)

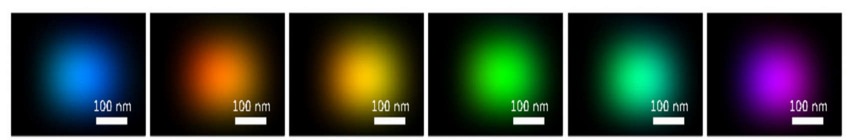
Synchrotron **R**adiation **W**orkshop

- C library for wavefront propagation

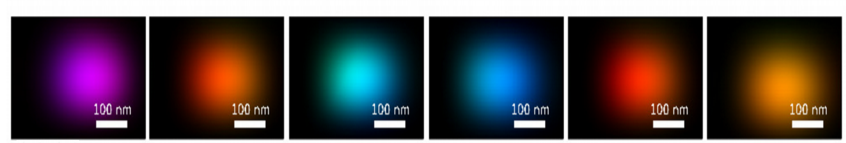
Wave **P**ropa**G**ator

- Python frontend for SRW
- Tutorial L. Samoylova (Thursday)





color: phase brightness: intensity Δt=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)

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

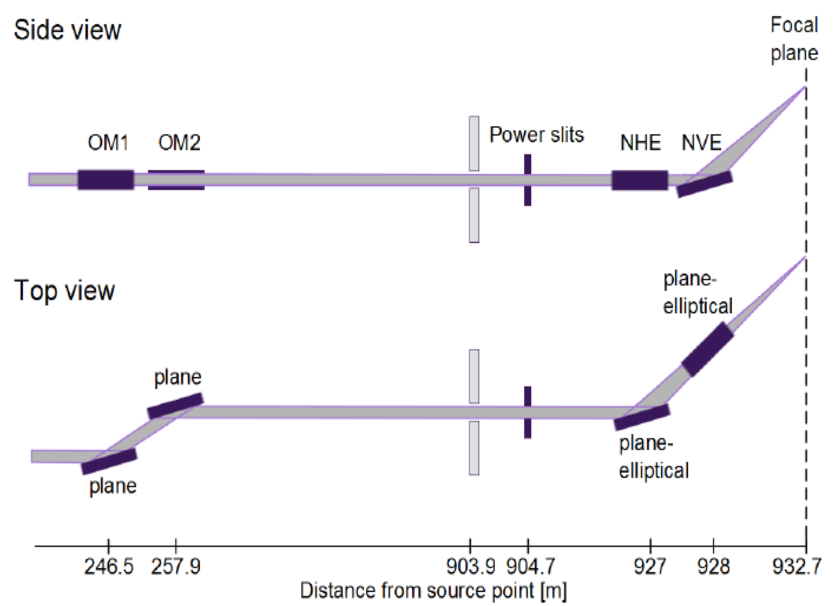
Wave propagation (WPG library)

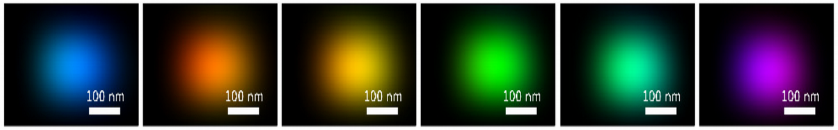
Synchrotron **R**adiation **W**orkshop

- C library for wavefront propagation

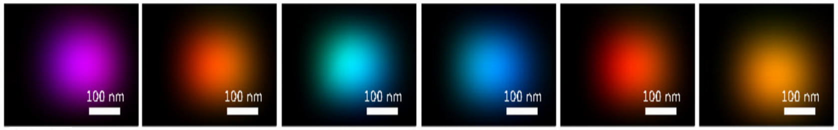
Wave **P**ropa**G**ator

- Python frontend for SRW
- Tutorial L. Samoylova (Thursday)





color: phase brightness: intensity Δt=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)

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

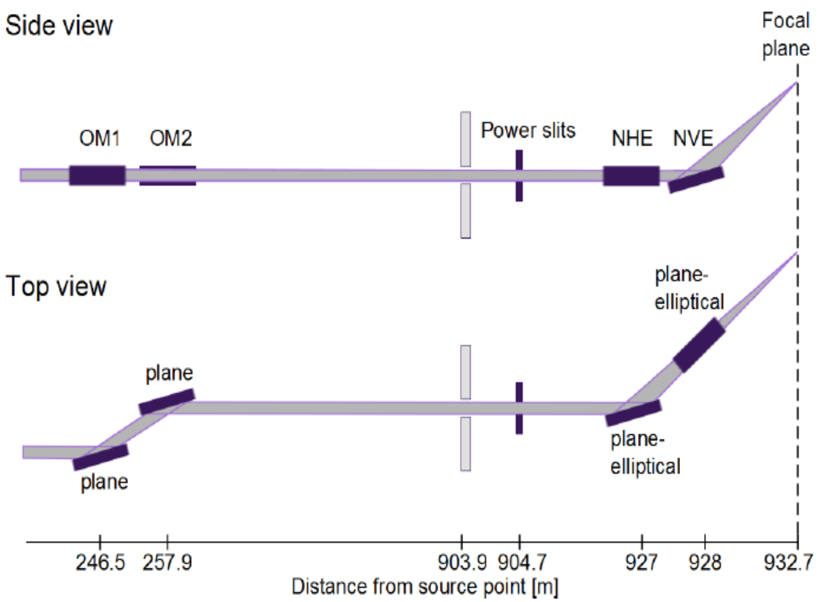
Wave propagation (WPG library)

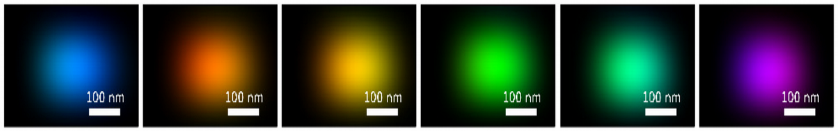
Synchrotron **R**adiation **W**orkshop

- C library for wavefront propagation

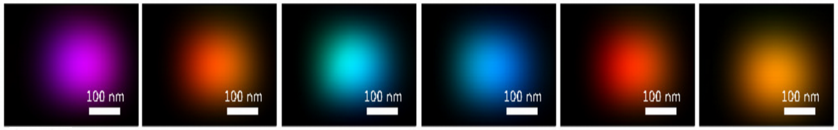
Wave **P**ropa**G**ator

- Python frontend for SRW
- Tutorial L. Samoylova (Thursday)





color: phase brightness: intensity Δt=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)

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

Photon-Matter interaction: Molecular Dynamics + Ab-initio electronic structure

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

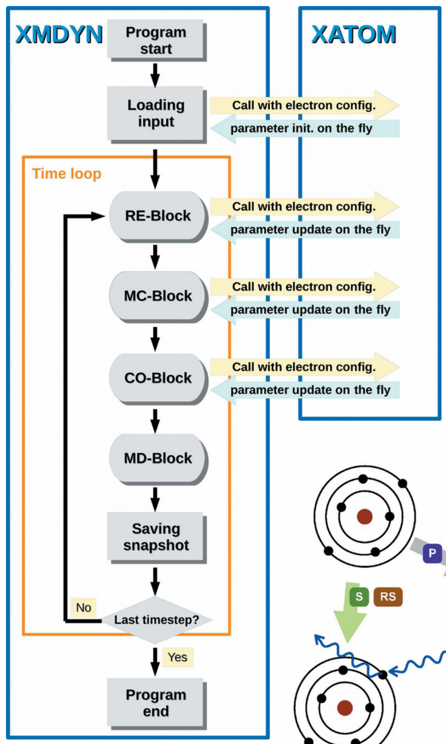
Son et al. Phys. Rev. A **83**, 033402 (2011)

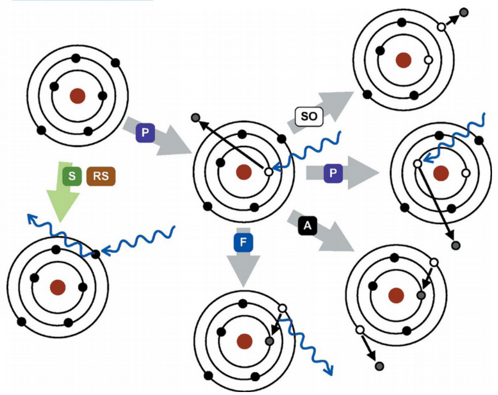
XMDYN & XATOM

- 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 $S(\mathbf{k}, t)$





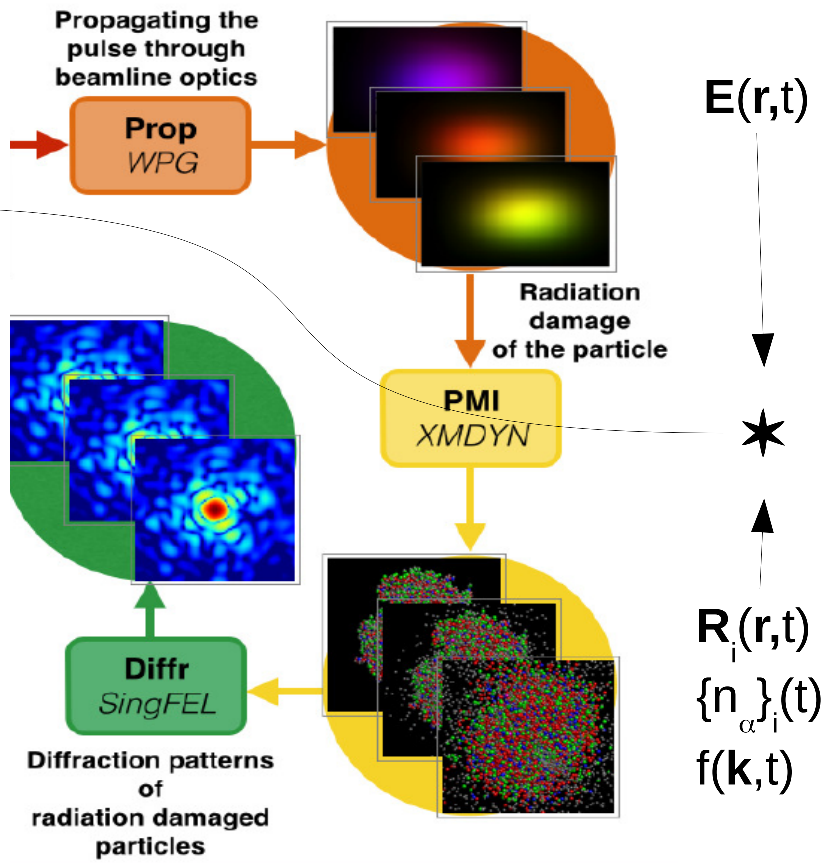
This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 654220

singFEL propagates photons scattered from the sample to the detector plane

Diffraction from single particles

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

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



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

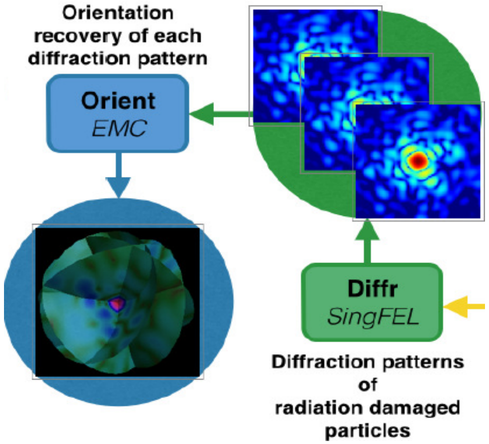
Electron density reconstruction from simulated diffraction patterns

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)

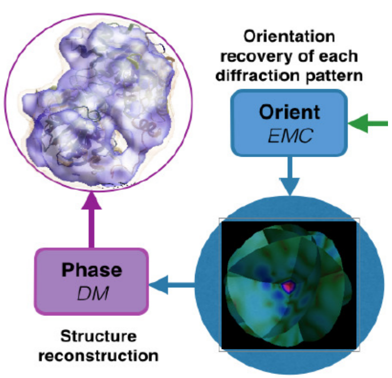


This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 654220

Electron density reconstruction from simulated diffraction patterns

Phase retrieval for electron density reconstruction

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

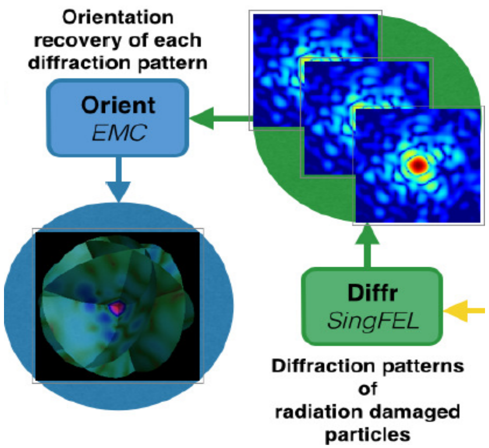


Orientation of 2D diffraction patterns into a 3D diffraction volume

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

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

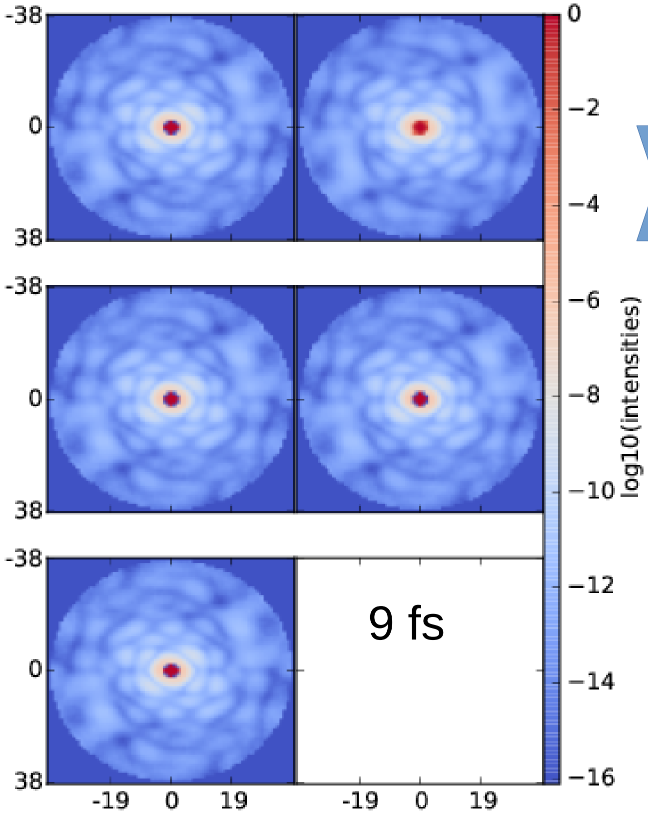
Yoon et al. Scientific Reports **6** 24791 (2016)

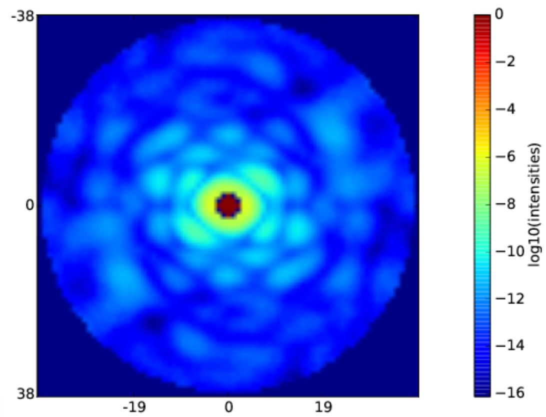


This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 654220

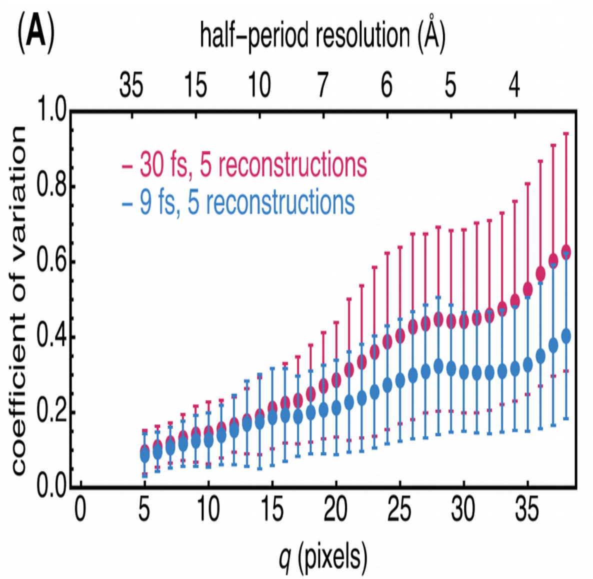
Quantifying 3D diffraction volume consistency: The coefficient of variation

Each run starts from a new, random initialization





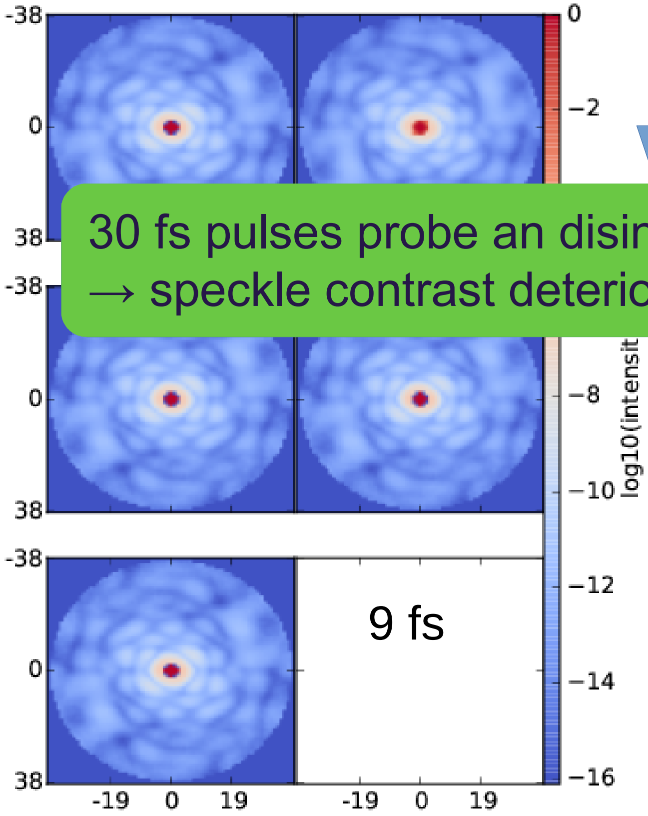
$$\sigma(\mathbf{q}) = \frac{\sqrt{\left\langle \left| I_n(\mathbf{q}) - \langle I_n(\mathbf{q})\rangle_n \right|^2 \right\rangle_n}}{\langle I_n(\mathbf{q})\rangle_n}$$

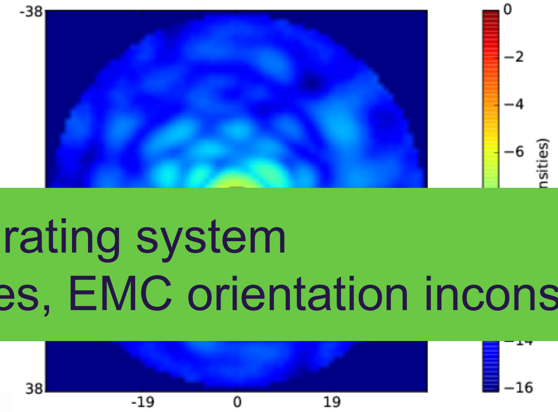


This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 654220

Quantifying 3D diffraction volume consistency: The coefficient of variation

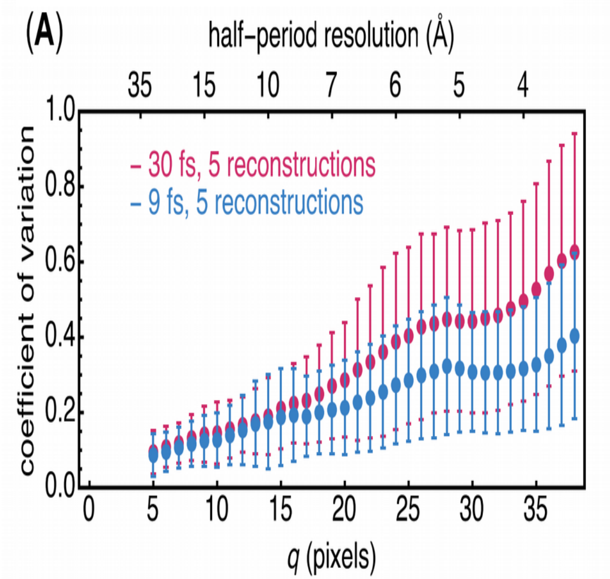
Each run starts from a new, random initialization





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

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



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

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.**

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

EUCALL

Acknowledgements

L. Samoylova, T. Rueter

M. Yurkov, E. Schneidmiller

Z. Jurek, B. Ziaja, R. Santra

C.H. Yoon

N.D. Loh

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