

EUCALL Mid-Term Review - WP 4

Adrian P. Mancuso - WPL



LUND UNIVERSITY



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





Outline

- Main WP objectives
- Main WP achievements
 - Software developments in SIMEX
 - Scientific applications (including extensions from proposal)
- Upcoming Milestones and Deliverables
- Outlook: SIMEX++



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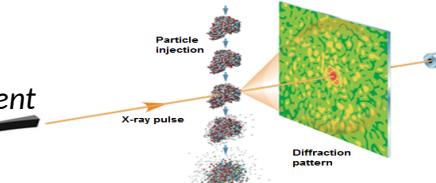
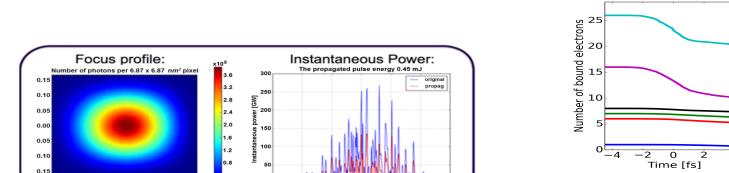
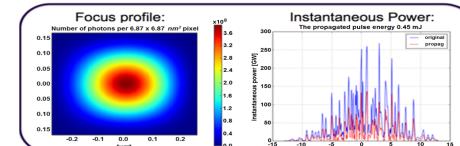
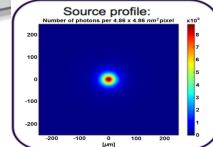
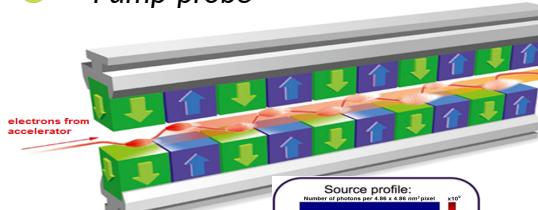
SIMEX' objective

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

- Yoon et al. Scientific Reports **6** 24791 (2016)
- Fortmann-Grote et al. NOBUGS (2016)
- Fortmann-Grote et al. SPIE Proceedings (2017)

Photon Source

- XFEL
- Synchrotron
- Optical Laser
- Pump-probe



Target/Sample

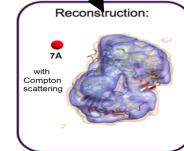
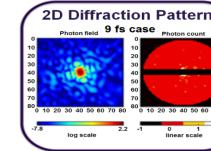
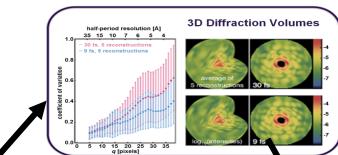
- Atoms, molecules, clusters
- Solids, surfaces
- Liquids
- Plasmas

Diagnostics

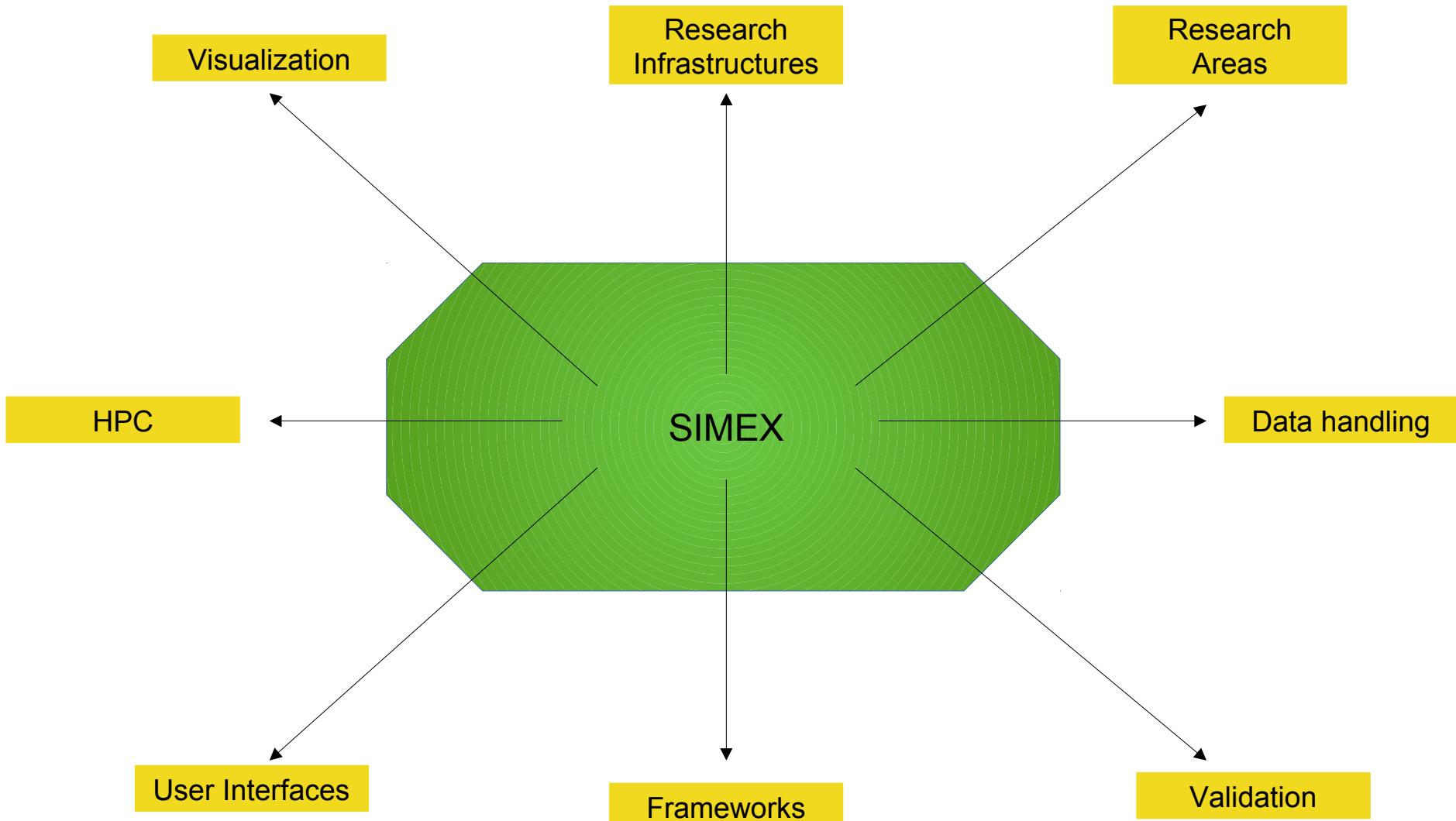
- Spectroscopy
- Diffraction
- Scattering

Photon Data Analysis

- Structure determination
- Electronic structure
- Transport
- Relaxation & Thermodynamics



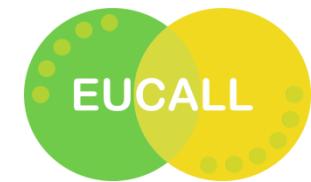
The dimensions of SIMEX



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Timeline

Software development

M1: Single modules interoperable

M2: First example simulation

M3: Simulations interoperable

50%

M4: Tested and documented simulation code

10%

Reports & data generation

D1: Short pulse laser matter interaction software

D2: Long pulse laser matter interaction software

2016

D3: Interoperability of simulation workflows

70%

D4: Generation of coherent scattering data

50%

2017

D5: Testing & validation

20%

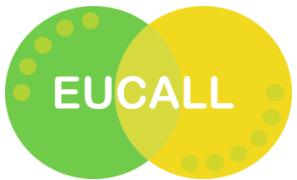
2018



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Publications out of SIMEX

- C. Fortmann-Grote et al., *Start-to-end simulation of single particle imaging using ultra-short pulses at the European X-ray Free Electron Laser*, IUCrJ (submitted)
- C. Fortmann-Grote et al., *Simulations of ultrafast x-ray laser experiments*, SPIE Optics & Optoelectronics Conference Proceedings, Prague (2017)
- C. Fortmann-Grote et al., *SIMEX: Simulation of Experiments at Advanced Light Sources*, in “New Opportunities for Better User Group Software” Conference Proceedings, 29 (2017); doi:10.17199/NOBUGS2016.21 (published May 2017)
- E. Zenker et al., *Alpaka – An Abstraction Library for Parallel Kernel Acceleration* 2016 IEEE International Parallel and Distributed Processing Symposium Workshops, (IPDPSW) 00: 631-640 (2016); doi: <https://doi.org/10.1109/IPDPSW.2016.50>
- E. Zenker et al., *Performance-Portable Many-Core Plasma Simulations: Porting PICoNGPU to OpenPower and Beyond*, Lecture Notes in Computer Science, 9945: 293-301 (2016); doi: http://dx.doi.org/10.1007/978-3-319-46079-6_21

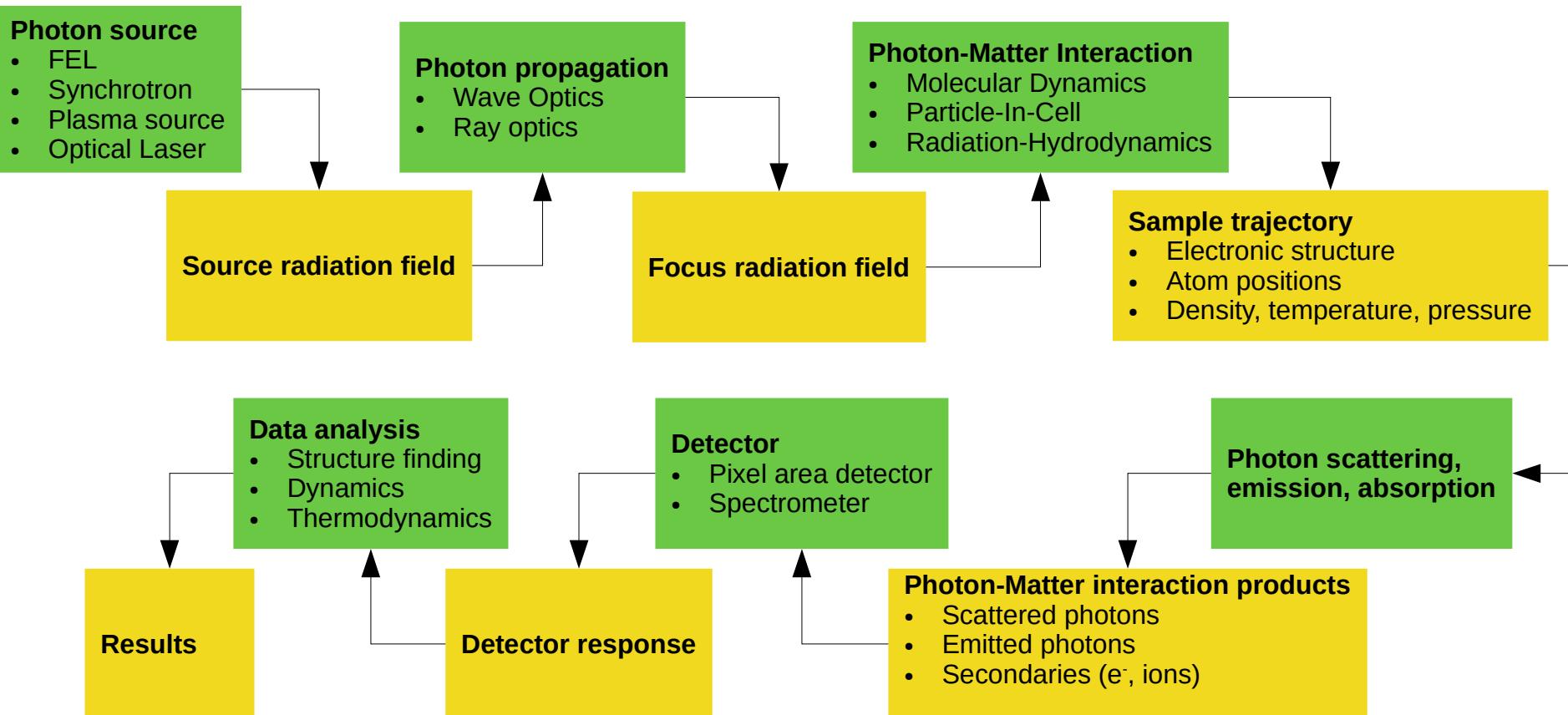


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SIMEX provides user interfaces and data formats for start-to-end photon experiment simulations



Calculators: Scriptable (python) interfaces to advanced simulation codes
 Data interfaces using metadata standards



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Simulation codes in SIMEX

X-ray source	FAST Genesis/Ocelot Oasys	FEL FEL Synchrotron	M. Yurkov, E. Schneidmiller S. Reiche, G. Geloni et al. L. Rebuffi, M. Sanchez-Rio
Propagation	WPG/SRW Oasys	coherent wavefront prop. x-ray tracing	L. Samoylova, O. Chubar L. Rebuffi, M. Sanchez-Rio
Photon matter interaction	XMDYN & XATOM Esther Multi2D PIConGPU	Atoms, molecules, clusters 1D Rad-Hydro 2D Rad-Hydro 3D PIC	Z. Jurek, S. Son, R. Santra Colombier et al. (CEA) R. Ramiz et al. M. Bussmann et al.
X-ray diagnostics	SingFEL paraTAXIS XRTS SLADS CrystFEL/pattern_sim FEFF8.5	molecule, cluster scattering Plasma SAXS Plasma Compton/Thomson SAXS, WAXS Crystal diffraction EXAFS, XANES	C.H. Yoon T. Kluge et al. G. Gregori, C. Fortmann-Grote Chen et al. T. White et al. (CFEL) J.J. Rehr et al. (U Washington)
Detector simulation	X-CSIT, Karabo	2D Pixel detectors	T. Rueter, A. Joy
Analysis/Reconstruction	EMC DM	Pattern orientation Phasing	N.D. Loh N.D. Loh



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SIMEX is developed as an opensource project on github

The screenshot shows a dual-monitor setup. The left monitor displays the GitHub organization page for "eucall-software" (<https://github.com/eucall-software>). The right monitor displays the "Travis CI" build status for the "simex_platform" repository (https://travis-ci.org/eucall-software/simex_platform).

GitHub Organization Page (Left Monitor):

- Table Of Contents:**
 - Users Manual
 - Indices and tables
 - Acknowledgements
 - Introduction
 - Installation
 - From sources
 - Download
 - Software dependencies
 - Building
 - Configuration via cmake
 - Troubleshooting
 - Building the library
 - Installation on
 - Binary packages
 - Docker
 - Getting started
 - Example tests
 - Updating docker container
 - Environment settings
 - Testing
 - Usage
 - Contribute
 - Support
 - License
 - Reference Manual
- This Project:**
 - simex optics
 - As an example
 - The x-ray source
 - simex Interactions
 - The simulation
 - Installations
 - From scratch
 - Downloads
 - First observation
 - git

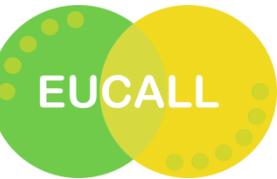
Travis CI Build Status (Right Monitor):

The Travis CI page shows the build status for various branches of the "simex_platform" repository.

Branch	Last Build Status	Last Commit	Build History	Build Grid
master	passed (#280)	59ceb39	43 builds	Green (✓) across all stages
hydro	failed (#427)	ad98d82	48 builds	Red (✗) across all stages
develop	passed (#423)	081c8d5	125 builds	Mixed: Red (✗), Green (✓), Yellow (⚠)
pattersim	passed (#422)	538580e	2 builds	Green (✓) across all stages
doc	passed (#288)	0b52e1f	30 builds	Mixed: Red (✗), Green (✓), Yellow (⚠)
feff	passed (#183)	f34d62d	16 builds	Mixed: Red (✗), Green (✓), Yellow (⚠)
xrt Hydro Integration	passed (#92)	a7b8499	3 builds	Green (✓) across all stages

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Remaining tasks in FY2

Task	Description	Assignee(s)	Data Deliverable	D	M
4.2.2.1	XFEL source	Carsten	Source field distribution $E(x,y,t)$	4.3	4.2, 4.3
4.2.2.2	Synchrotron source	ESRF	Source Intensity distribution	4.3	4.3
4.2.2.3	Plasma x-ray source	HZDR/ELI	Source Intensity / field distribution	4.3	4.3
4.2.2.4	Coherent wavefront propagation	Carsten	Focus field distribution, caustic	4.3	4.2, 4.3
4.2.2.5	X-ray tracing	Richard/Carsten	Focus intensity distribution, caustic	4.3	4.3
4.2.2.6	PMI: Rad. damage in biosamples	Carsten	Molecular trajectory ($R(t), f(q,t)$)	4.3	4.2, 4.3
4.2.2.7	PMI: Plasmas	HZDR	PIC dump	4.3	4.3
4.2.2.8	PMI: Shock compression	Richard	Rad-hydro ($\rho(t), T(t), p(t)$)	4.3	4.3
4.2.2.9	Signal from thin sample	HZDR Carsten Carsten Carsten	SAXS image from underdense plasma Diffraction patterns from biomolecule Crystal diffraction pattern Solution scattering SAXS image	4.3, 4.4 4.3, 4.4 4.3, 4.4 4.3, 4.4	4.3 4.2, 4.3 4.3 4.3
4.2.2.10	Signal from thick sample	Richard HZDR/ELI	XAFS shock compressed matter SAXS image from overdense plasma	4.3, 4.4 4.3, 4.4	4.3 4.3



M36 deliverables and milestones

- **D4.5/Task 4.3.1: , Benchmarking, testing, validation, example workflow**
 - Validation against Virus data (AMO@LCLS)
 - Validation against C60 data ([CXI@LCLS](#))
 - Iterative optimization workflow: Target design for dynamic compression experiments
 - Performance benchmarks for selected simulation codes
- **Task 4.3.2: HPC, data management, data analysis**
 - SIMEX codes run on modern HPC infrastructures including GPU clusters
 - Deployment options: source tarballs, binary packages, docker images
 - Webbased SIMEX frontend under development

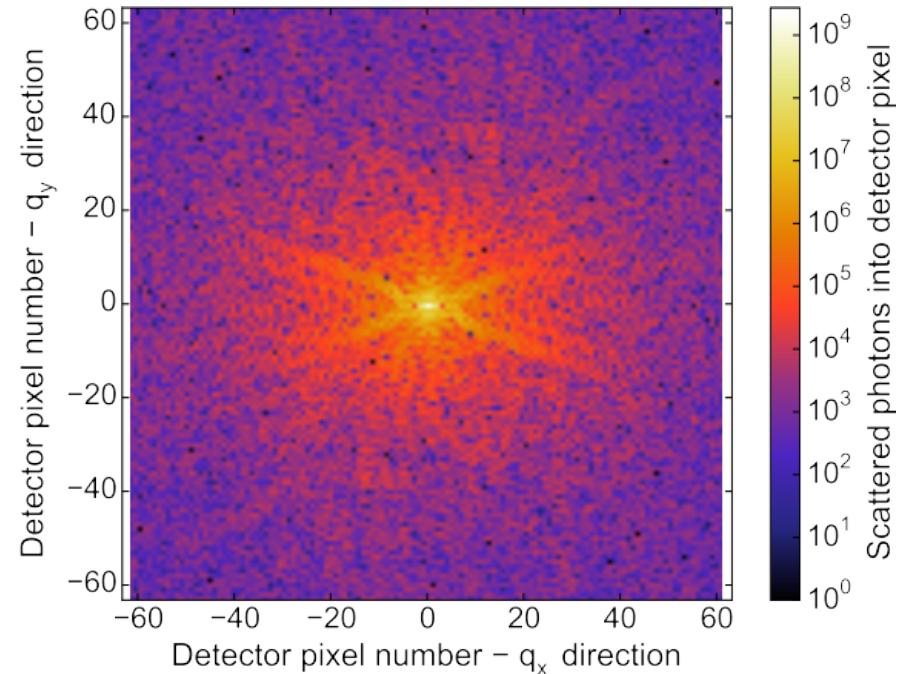
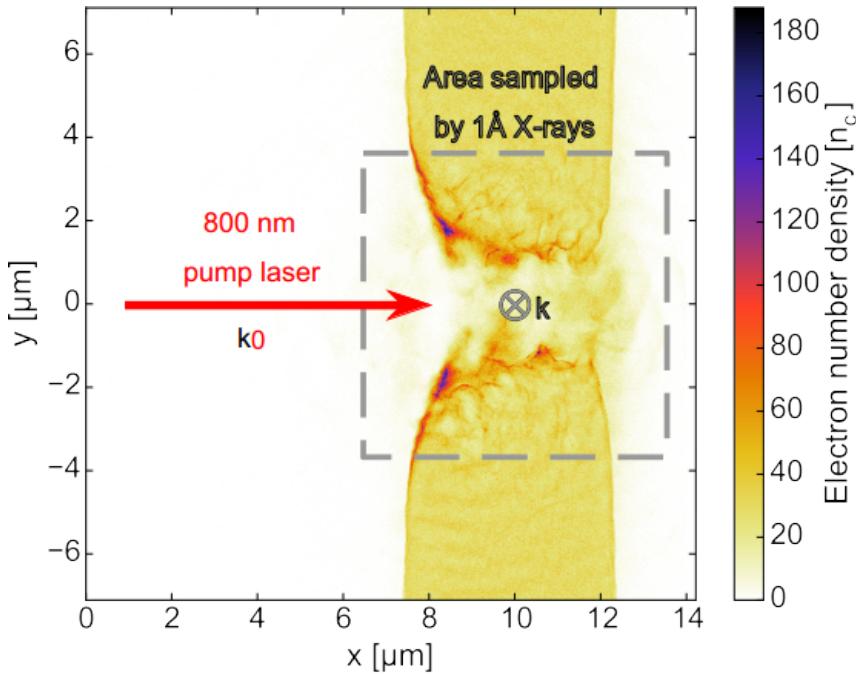


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SAXS on high-power laser driven solid targets



- Target: 5 μm cryogenic hydrogen
- Laser: 800 nm, 30 fs, 105 TW
- Probe: 1 \AA , 10^{12} photons / $50 \mu\text{m}^2$ focus
- 2D PIC simulation
- R.Mishra, Phys. Plasma **20**, 072704(2013).

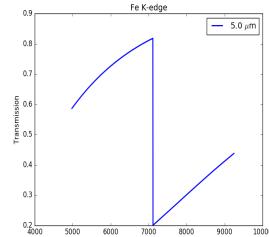
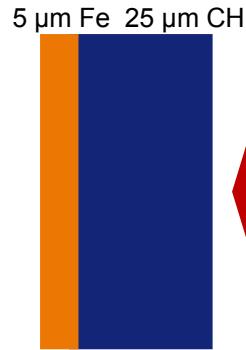
- SAXS pattern 134 fs after laser pulse
- Detector distance 93 cm
- Avg. photon count: $10^{5..6}$ / pixel
- SAXS simulation: paraTAXIS code



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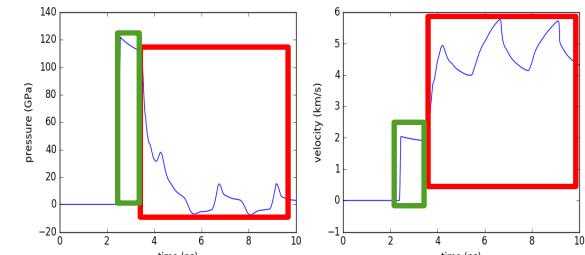
SIMEX assists in target design optimization for dynamic compression experiments at ESRF



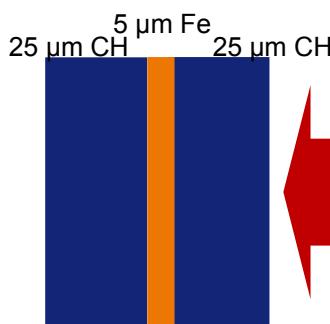
```
# Create parameters.
parameters = EstherPhotonMatterInteractorParameters(
    number_of_layers=2,
    ablator="CH",
    ablator_thickness=25.0,
    sample="Iron",
    sample_thickness=5.0,
    window=None,
    window_thickness=0.0,
    laser_wavelength=1064.0,
    laser_pulse='flat',
    laser_pulse_duration=4.0,
    laser_intensity=1.98,
    run_time=10.0,
    delta_time=0.01
)
```

1064 nm
4 ns
1.98 TW/cm²

→ Setup calculation parameters → Run calculation → Analyze results



Initial sample target design.



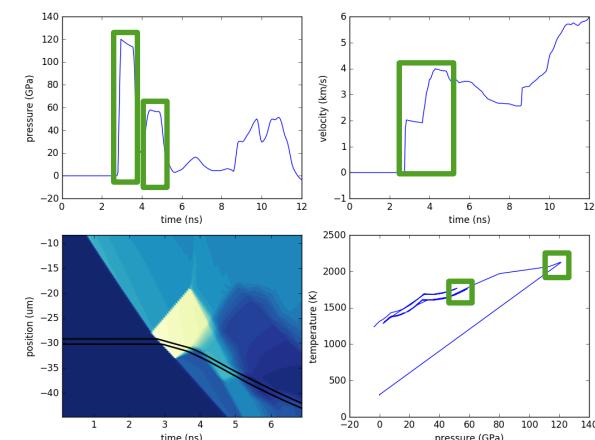
1064 nm
4 ns
1.98 TW/cm²

← Re-design (add window layer to confine target) ←

```
# Create new experiment from previous with update.
new_parameters = EstherPhotonMatterInteractorParameters(window='CH', window_thickness='25.0'
    read_from_file='Simulations/Iron/1')

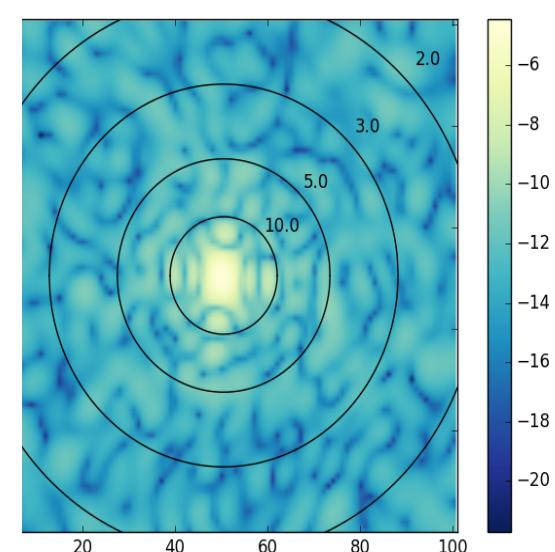
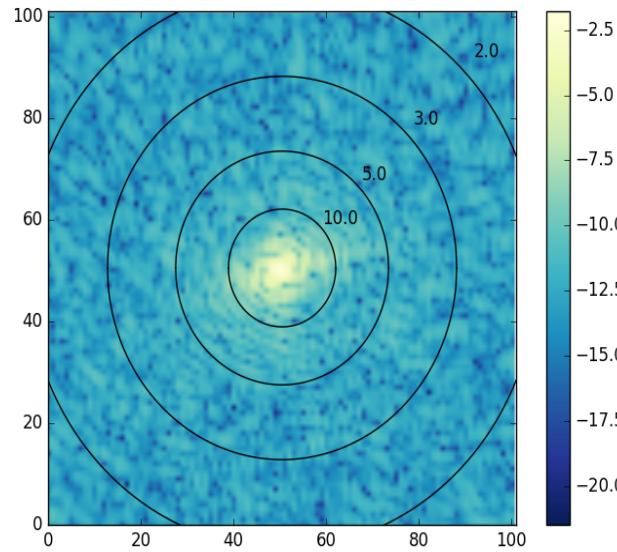
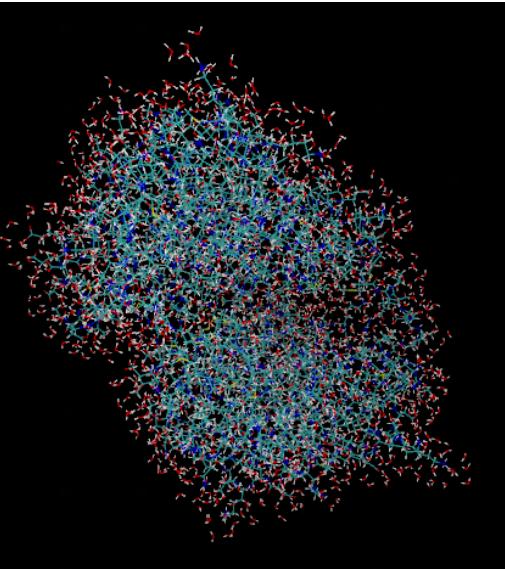
experiment = EstherExperimentConstruction(parameters=new_parameters,
    esther_sims_path=self._simdir,
    sim_name=parameters.sample)
```

→ Update calculation parameters → Run calculation → Analyze results -

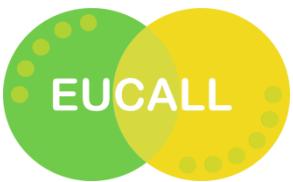


Single particle imaging of biomolecules

$2\text{NIP} + 3\text{\AA H}_2\text{O}$



2NIP imaging at various pulse duration: C. Fortmann-Grote et al. (under review).



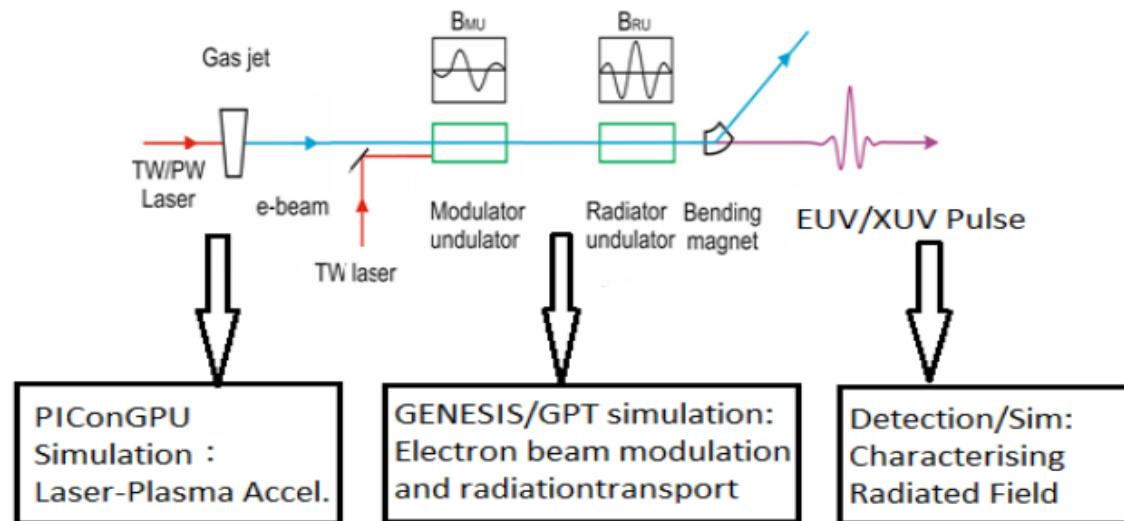
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Laser-plasma acceleration based x-ray source

- Simulate laser wakefield acceleration (PIC)
- Feed electrons into FEL simulation code
- New and hot topic, extension of EUCALL proposal



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Summary and Conclusions

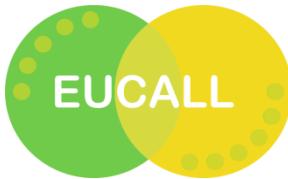
- SIMEX achieved Milestones and Deliverables up to date.
- On track for M24 Ms&Ds.
- M36 Ms&Ds are in progress.
- simex_platform is exploited for scientific output.
- Future plans for SIMEX are beginning to emerge.



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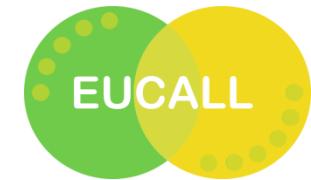




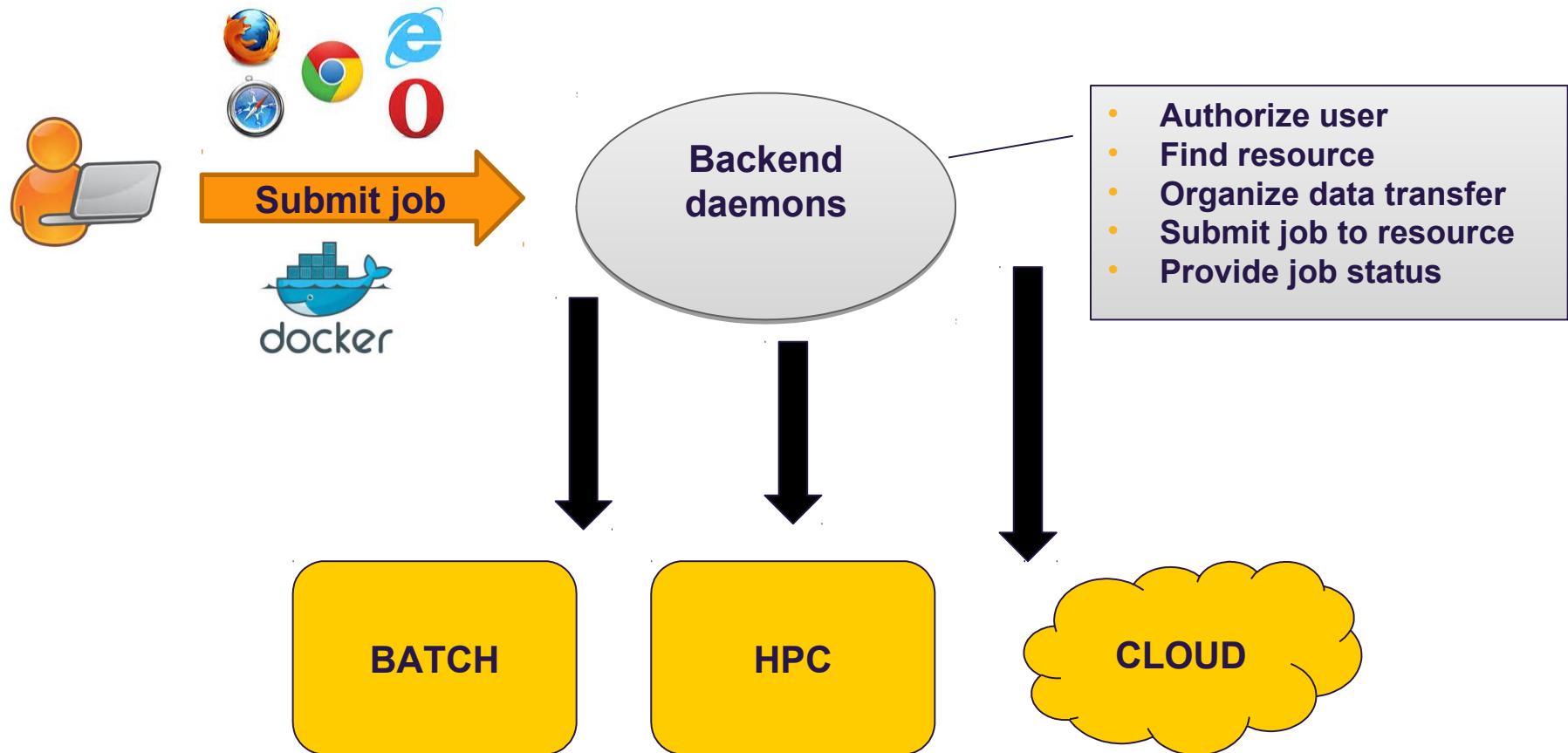
Benchmarking Experiments Against Modeling and¹⁷ Simulation (BEAMS)

- Close the loop between experiments and theory by benchmarking experiments against detailed simulation in the photon sciences
- Include other “beam-like” fields: e.g. neutron, astro, HEP
- modeling experiments feasible at today’s facilities and benchmarking the results of experiments to the modeling
 - improved understanding of physics
 - more accurate forward models of physical phenomena
- Include rapid data analysis
 - Feedback for potentially data hungry experiments.
- Potential (natural) partners
 - EUCALL: SIMEX , UFDAC
 - CFEL, ILL, MAX IV, ESS
 - Astronomy/Astrophysics groups, HEP community





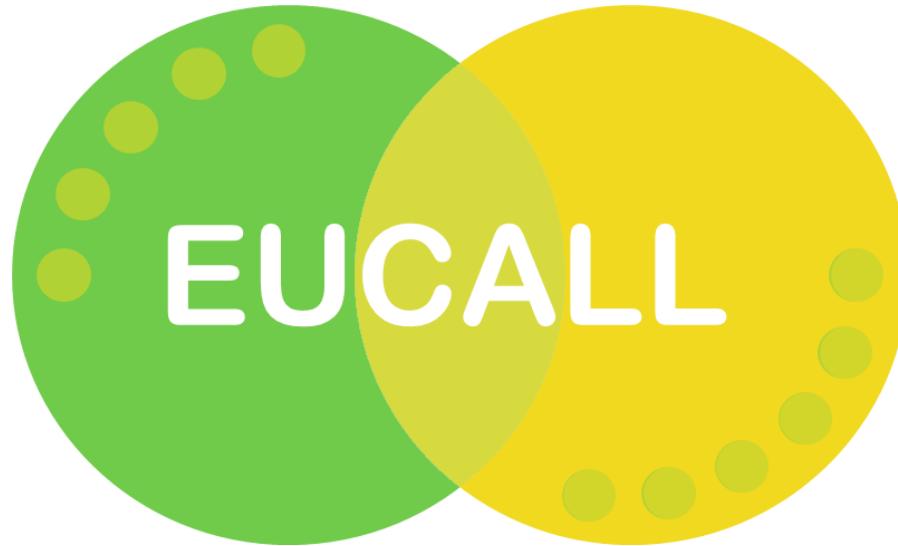
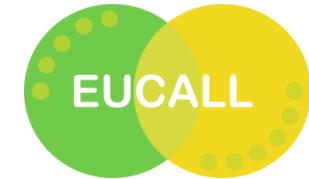
SIMEX as a Service



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Thank you for your attention

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