WP 5 - Virtual Neutron and X-ray Laboratory

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The 1st Annual Meeting of PaNOSC
WP5 face-2-face
Trieste, Nov. 7, 2019

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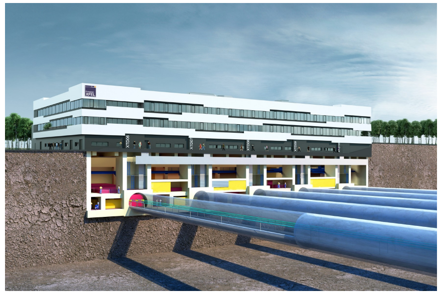
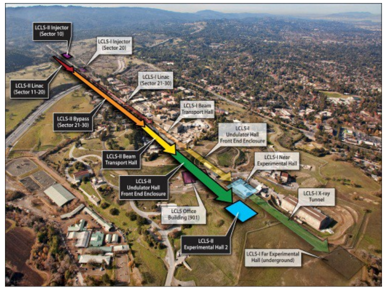
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823852.

Synchrotron radiation and free electron laser X-ray facilities provide new opportunities in investigating ultrafast (fs - ns) processes in complex systems

XFEL facilities



EuXFEL



LCLS

SACLA

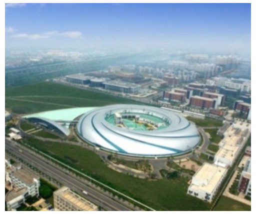
Synchrotron radiation facilities

ESRF

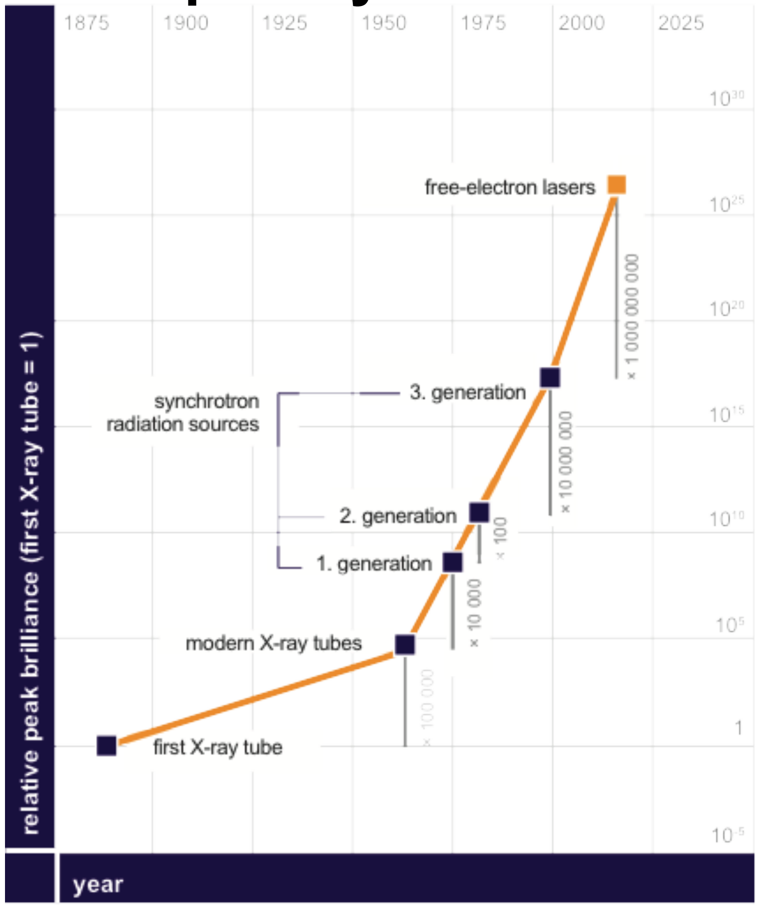
APS

Spring-8

PETRA 3



SSRF



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Start-to-end experiment simulations enable facility users and operators to ...

- Study impact of real-world error sources on experimental observables (isolated or in combination)
  - X-ray source fluctuations in time and space
  - Diffraction from optical elements, optical artifacts (mirror profile, slope error, lens material properties)
  - Radiation damage to components and samples
  - Incoherent scattering, dispersion
  - Detector geometry, misalignment, response
- Optimize instrument and experiment setups to maximize data quality
- Assess feasibility of proposed experiments (users, operators, reviewers)
- Teach students and new users to familiarize with the experiment
- Complement data analysis (inverse reconstructions <–> forward modeling)

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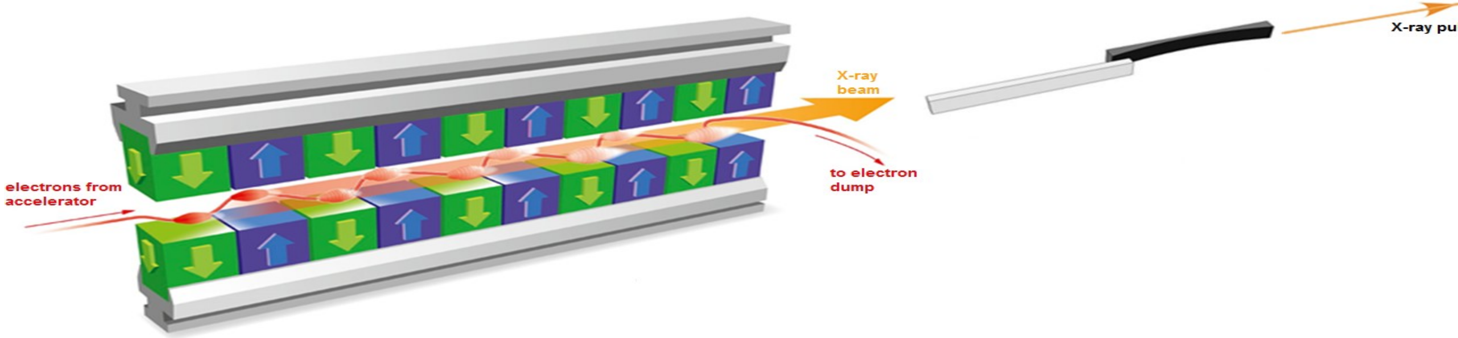
The key objective of SIMEX is to develop a simulation platform for users and facility operators to simulate experiments “from source to detector” at advanced light sources.

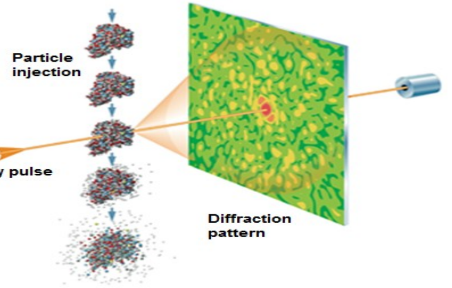
Photon Source
- *XFEL*
- *Synchrotron*
- *Op0cal Laser*

Photon propaga/on
- *Fully coherent*
- *Raytracing*
- *Hybrid*

Signal genera/on
- *Spectroscopy*
- *Diffrac0on*
- *Inelas0c scaAering*

Detector response
- *Pixel detectors*





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

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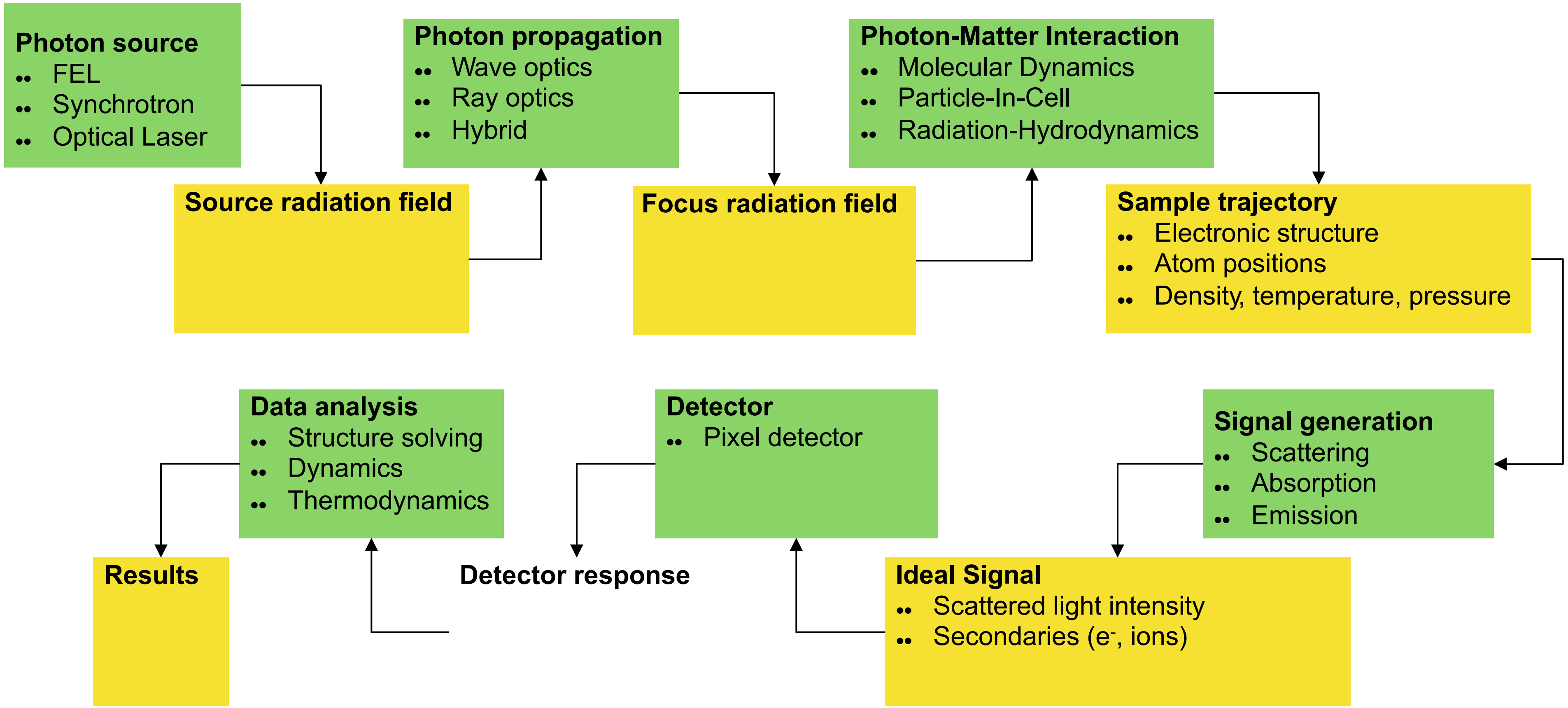
SIMEX provides user interfaces and data formats for start-to-end photon experiment simulations



Calculators: python APIs to advanced simulation codes Data interfaces based: open metadata standards: openPMD

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Interfaced simulation codes

X-ray source	FEL FEL Synchrotron	FAST Genesis/Ocelot Oasys	Yurkov, Schneidmiller (DESY) S. Reiche / G. Geloni et al. L. Rebuffi, M. Sanchez-Rio
Propagation	coherent wavefront prop. x-ray tracing	WPG/SRW Oasys	Samoylova, Buzmakov, Chubar L. Rebuffi, M. Sanchez-Rio
X-ray photon matter interaction	Atoms, molecules, clusters	XMDYN & XATOM MCMD HF/LDA	Z. Jurek et al. (CFEL) P. Ho et al (ANL) H. Quiney et al. (U Melbourne)
Optical photon matter interaction	1D Rad-Hydro 2D Rad-Hydro 3D PIC	Esther Multi2D PIConGPU	Colombier et al. (CEA) R. Ramiz et al. M. Bussmann et al. (HZDR)
Signal generation	molecule, cluster scattering Plasma SAXS Plasma Compton/Thomson Crystal diffraction EXAFS Diffraction (large systems)	SingFEL paraTAXIS XRTS CrystFEL/pattern_sim FEFF8L GAPD	C.H. Yoon (LCLS) T. Kluge et al. (HZDR) G. Gregori, CFG T. White et al. (CFEL) J.J. Rehr et al. (U Washington) J. C. E, S. N. Luo (PIMS China)
Detector simulation	2D Pixel detectors	X-CSIT, Karabo	T. Rüter et al. (XFEL)
Analysis/Reconstruction	Pattern orientation Phasing	EMC DM	N.D. Loh (Singapore)

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Simulation applications

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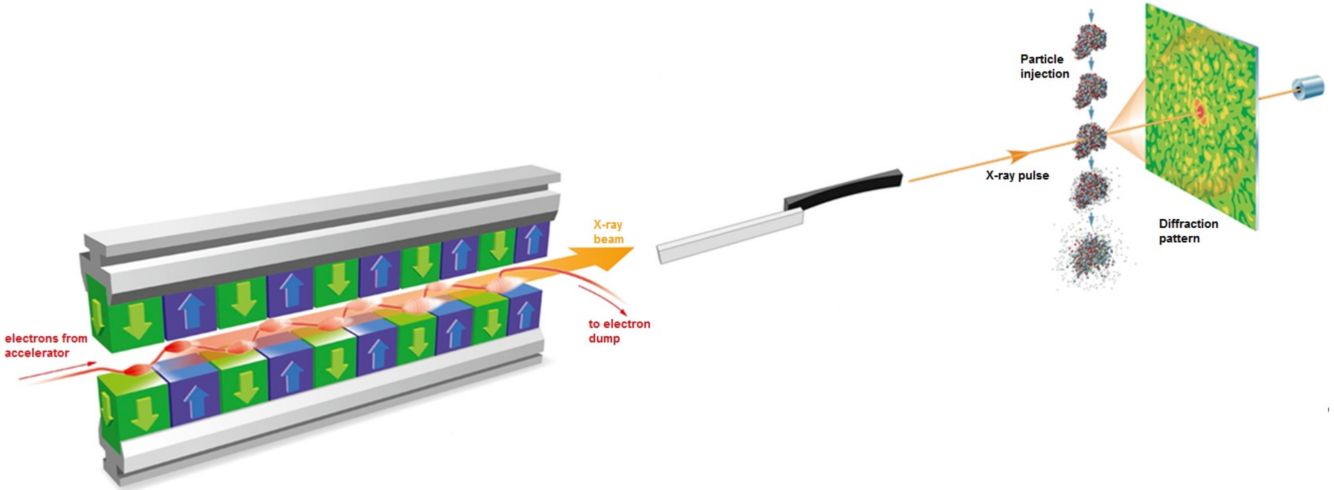
Instrument optimization example

- Simulation of single-particle imaging (SPI) at SPB-SFX instrument of European XFEL



- Coherent x-ray pulses (few fs, few 10^{11} photons/pulse) focused to few 100 nm beam diameter scatter from individual particles
  - (Bio-) Molecules, Clusters, Nanoparticles, Viruses, Cells
- Single-shot diffraction patterns ($10^{5..6}$) reveal 3D electron density after orientation and phasing (“computational lense”)
  - Allows structure determination of previously inaccessible molecules for biological and medical science

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Things that get in the way of SPI

- Radiation damage
  - Ionization: Coherent scattering ~$(N_{bound})^2$
  - Displacement: Loss of contrast due to randomly moving atoms
- X-ray beam fluctuations
  - temporal pulse shape
  - spectrum
  - pointing stability
  - fluence
- Sample position
- Background radiation
  - Compton scattering (as function of ionization)
  - Diffraction from optical elements in beamline
  - Detector noise
  - Sample atmosphere (solvent, contamination, clustering)

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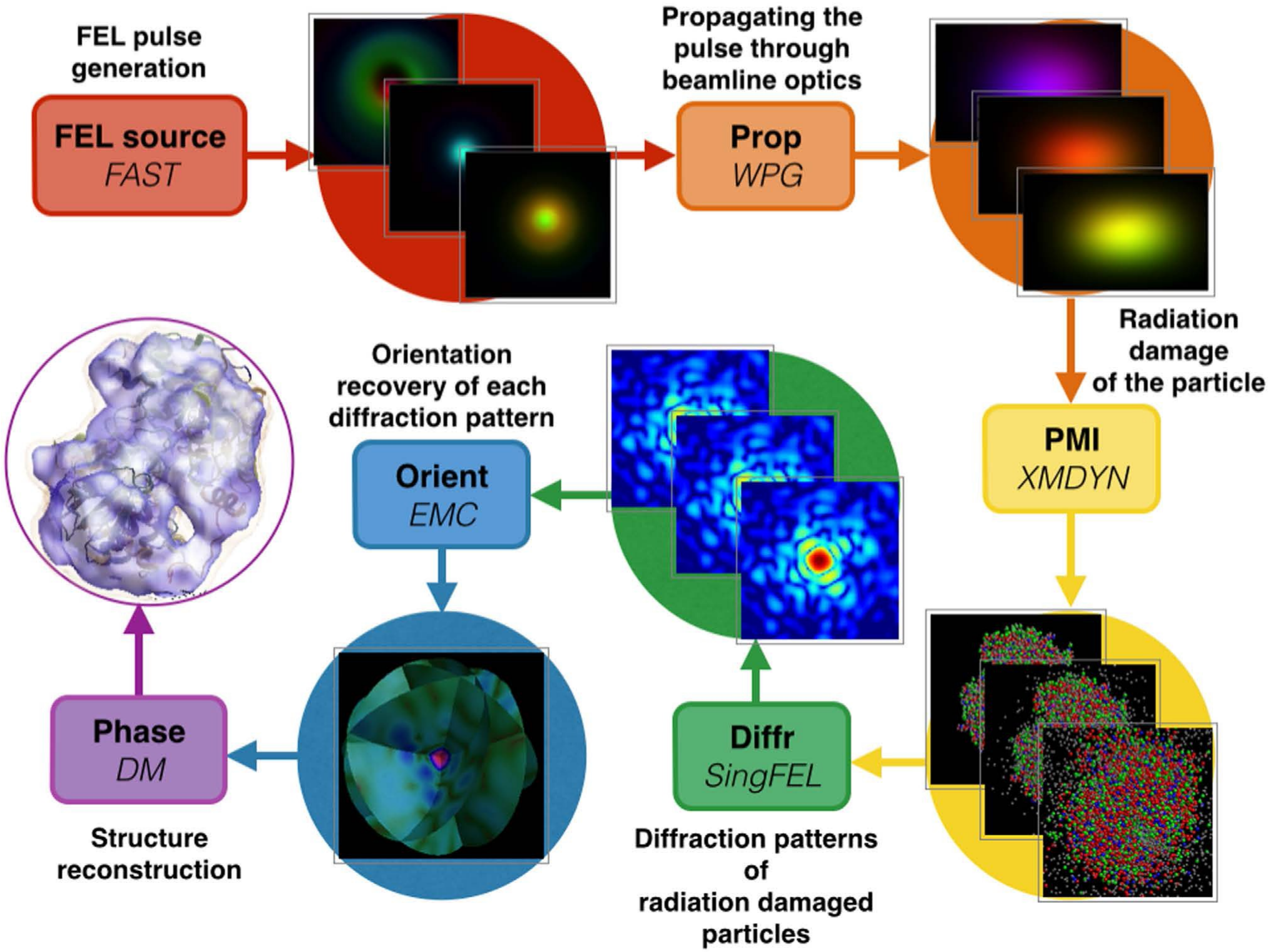

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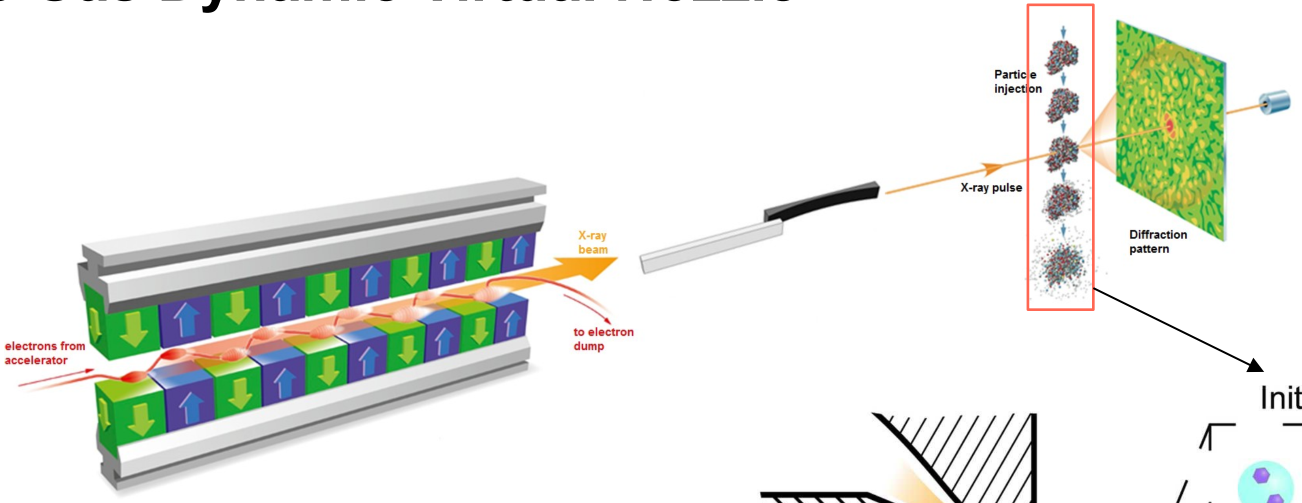
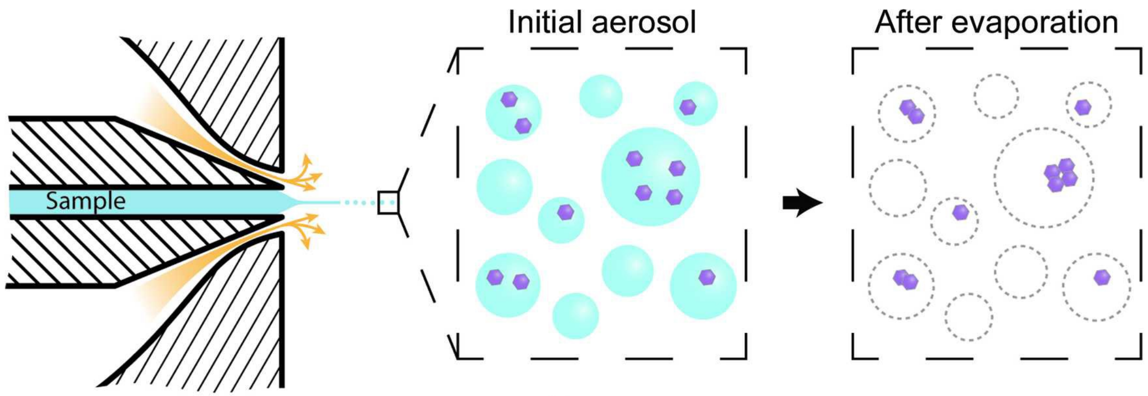
Solvated proteins are injected through the Gas Dynamic Virtual Nozzle





Up to which sample layer of thickness can people still successfully orient or phase the data?

Daurer et al., IUCrJ **4**, 251 (2017)

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Assessing the impact of water layer on diffraction pattern data

- Propagation of 5 keV 10 fs pulses through SPB-SFX beamline optics, 100 nm KB focusing
- Molecular Dynamics (MD) simulations of fixed protein in a water box
- Extract sample = protein + x Å water (x = 1...20)
- Simulate diffraction image from randomly oriented samples
- Measure “data quality” as function of x
- Neglected in this study:
  - Source fluctuations
  - Radiation damage
  - Clustering of molecules in same solvent droplet

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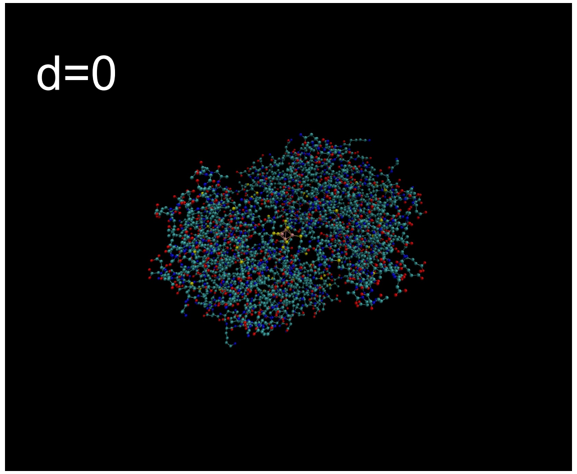

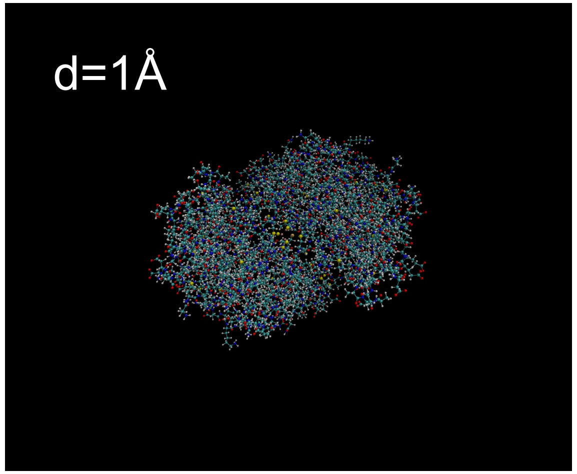

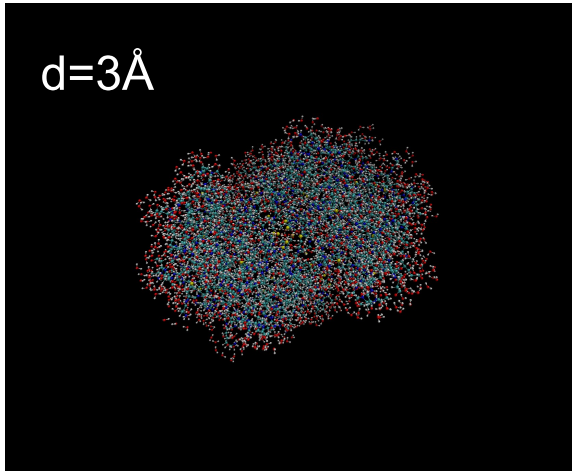

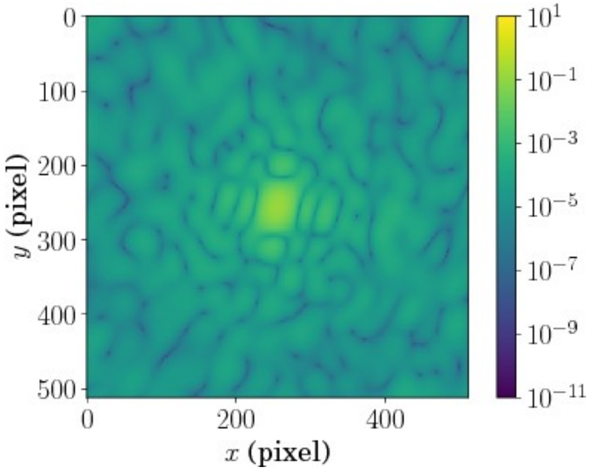

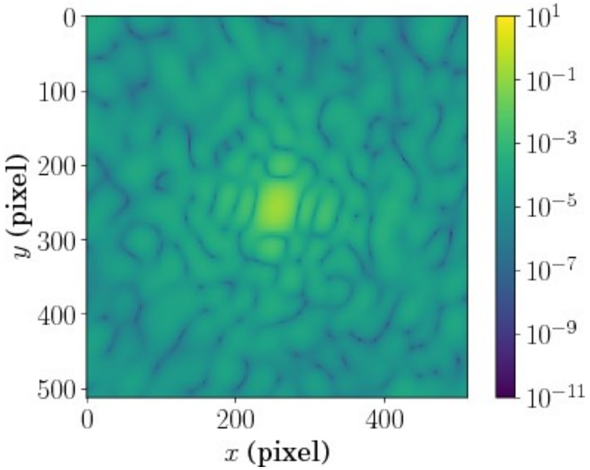

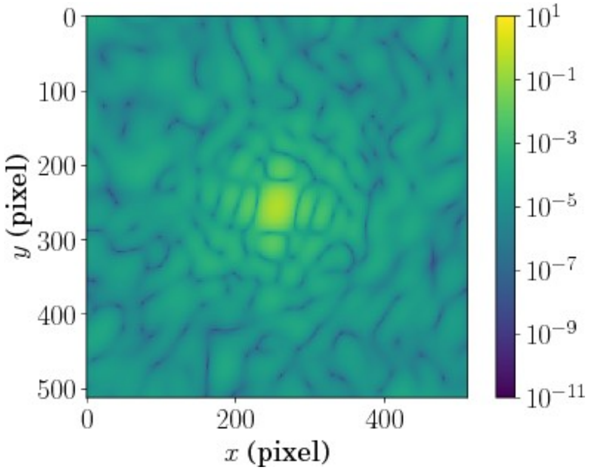

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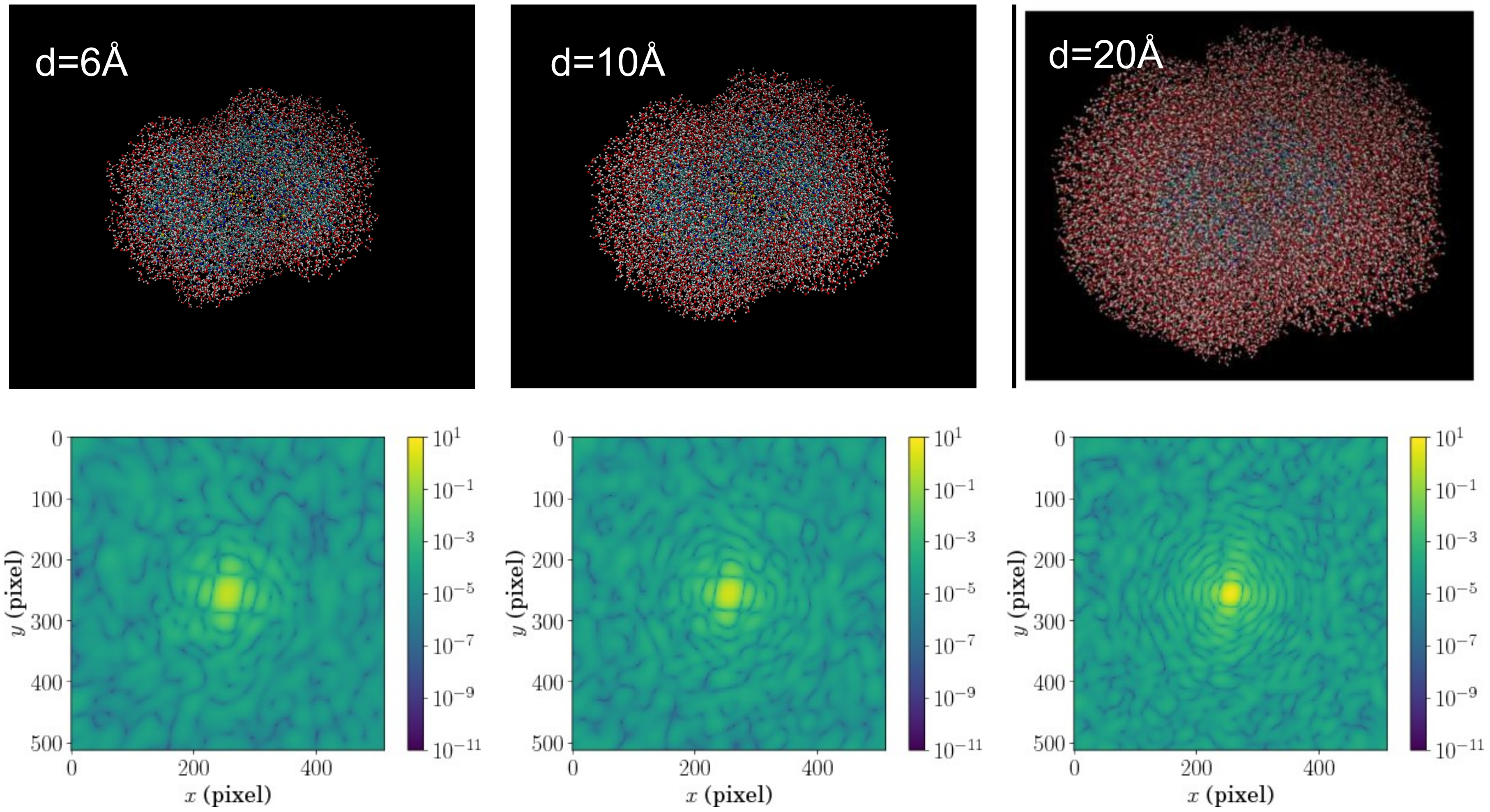

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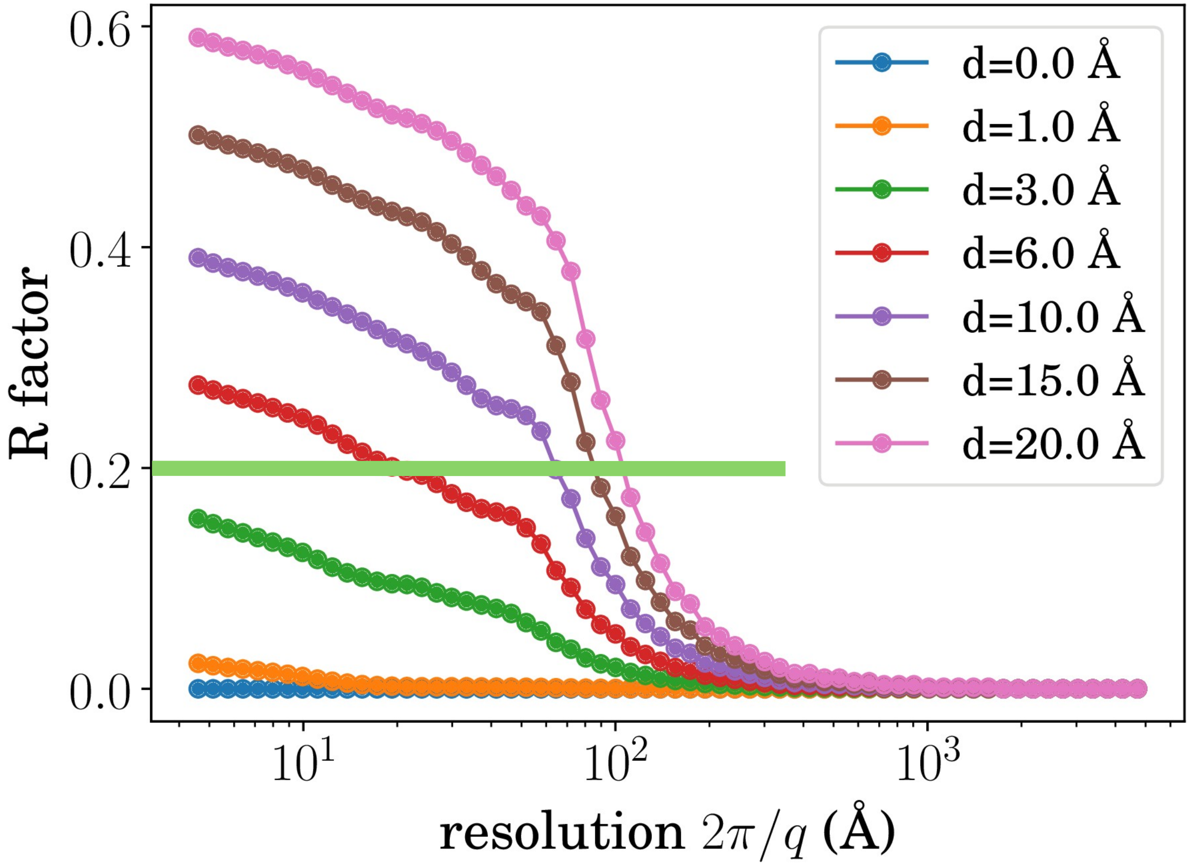
The R factor measures the quality of diffraction patterns. R < 0.2 indicates good data.

$$R(d) = \int_{Q<Q_{\max}(d)} \left| \frac{\sqrt{N_{\rm real}(\Omega)}}{\int_{Q'<Q_{\max}(d)} \sqrt{N_{\rm real}(\Omega')} d\Omega'} - \frac{\sqrt{N_{\rm ideal}(\Omega)}}{\int_{Q'<Q_{\max}(d)} \sqrt{N_{\rm ideal}(\Omega')} d\Omega'} \right| d\Omega,$$

$N_{real} \rightarrow d > 0$

$N_{ideal} \rightarrow d=0.0$



Presence of water layer of < 3 Å thickness is not adverse at a resolution of <10 Å length scale

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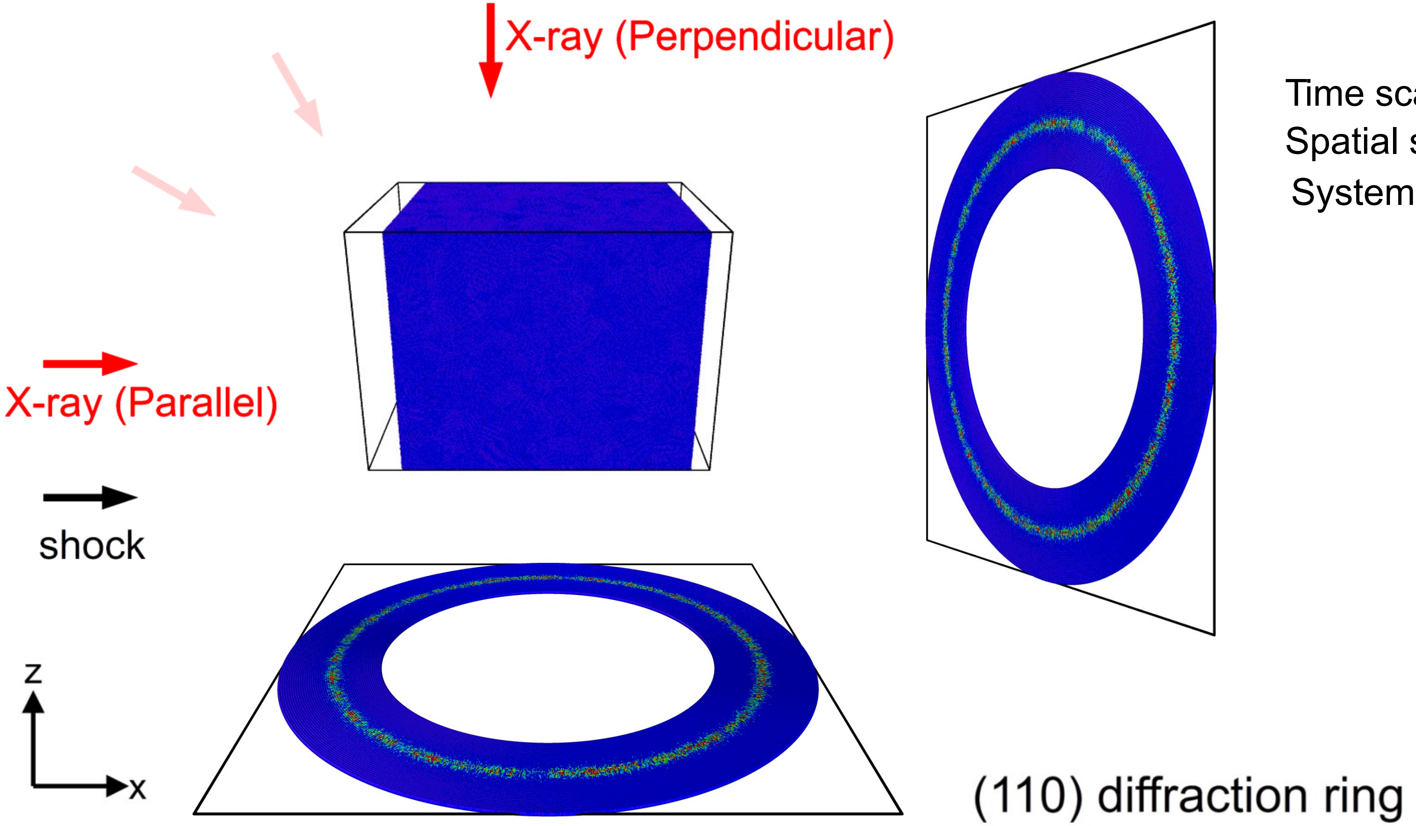
Methodology validation example

- Deducing density and strength of nanocrystalline diamond under shock compression for advanced light sources



Time scale: ps
Spatial scale: nm
System size: 19 million atoms

Y.Y. Zhang, M.X. Tang, Y. Cai, J.C. E, and S.N. Luo, *Journal of Synchrotron Radiation* 26, 413 (2019).

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Strength measurement under uniaxial compression

- Strength: the maximum differential stress that a material can support
- Definitions:
  - $\sigma_{\mathrm{P}} = \dfrac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3}$: equivalent hydrostatic pressure
  - $t = \sigma_{xx} - \dfrac{\sigma_{yy} + \sigma_{zz}}{2}$: differential stress

How to make *in situ* measurements of *t* under shock compression?

Y.Y. Zhang, M.X. Tang, Y. Cai, J.C. E, and S.N. Luo, *Journal of Synchrotron Radiation* 26, 413 (2019).

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$$d_{\mathrm{m}}(hkl) = \underline{d_{\mathrm{P}}(hkl)}[1+(1-3\cos^2\psi)\,\underline{Q(hkl)}]$$

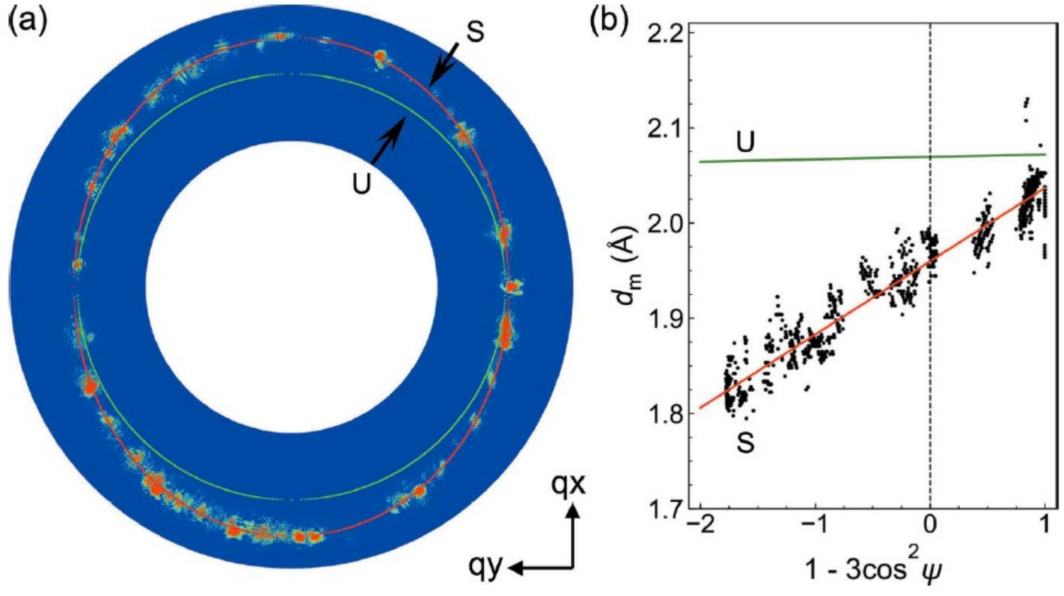
- ► d_{m} measured d-spacing
- ► d_{P}: d-spacing under σ_P

$$Q(hkl) = \frac{t}{6}\{\alpha[G_{\mathrm{R}}^{X}(hkl)]^{-1} + (1-\alpha)[G(V)]^{-1}\}$$

- ► G_R^X shear modulus under Reuss assumption
- ► $G(V)$: shear modulus under Voigt assumption
- ► α: weight factor

$$t = 6G\langle Q(hkl)\rangle f(x,\alpha)$$

- ► $f(x,\alpha) \approx 1.0$ as assumption
- ► G: arithmetic mean of $G(R)$ & $G(V)$



Singh, A. K. (1993). J. Appl. Phys. 73, 4278–4286.

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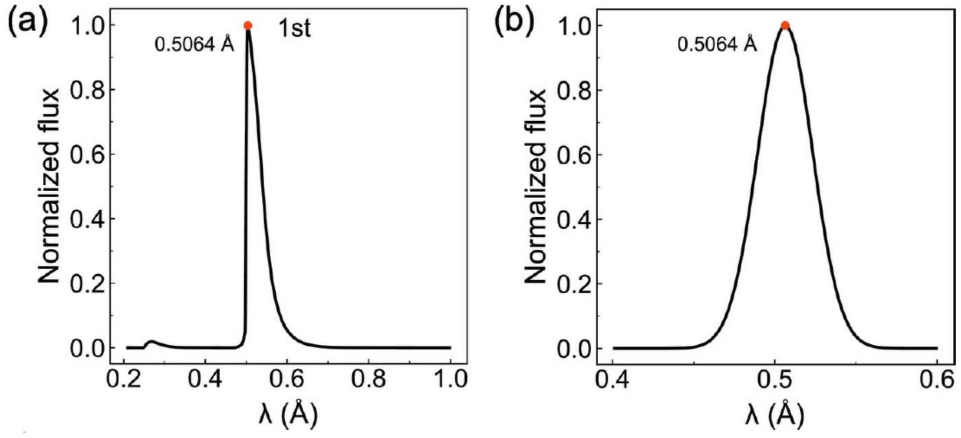
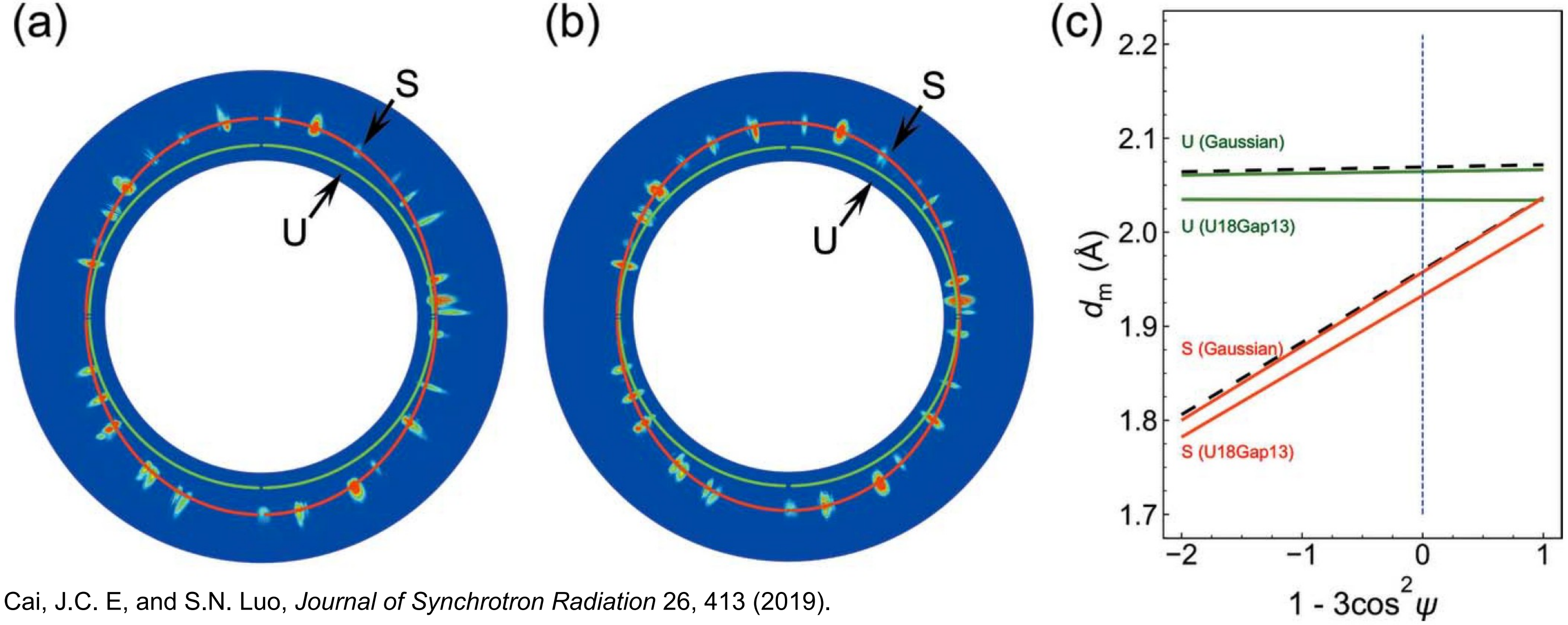


- Slope: strength, not affected by the spectrum width or symmetry
- Intercept: density, affected by the asymmetry of the undulator x-ray spectrum



Y.Y. Zhang, M.X. Tang, Y. Cai, J.C. E, and S.N. Luo, *Journal of Synchrotron Radiation* 26, 413 (2019).

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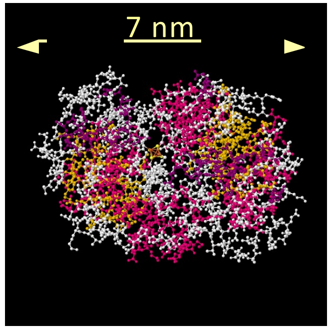
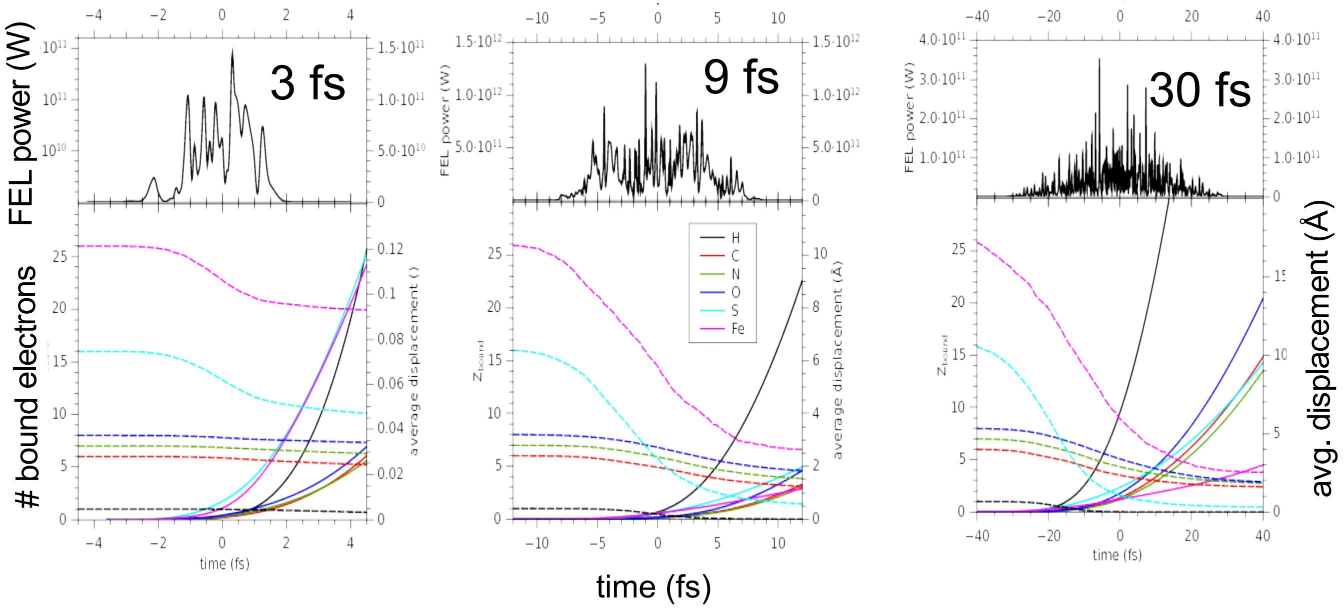
Identify optimal pulse duration for small protein imaging



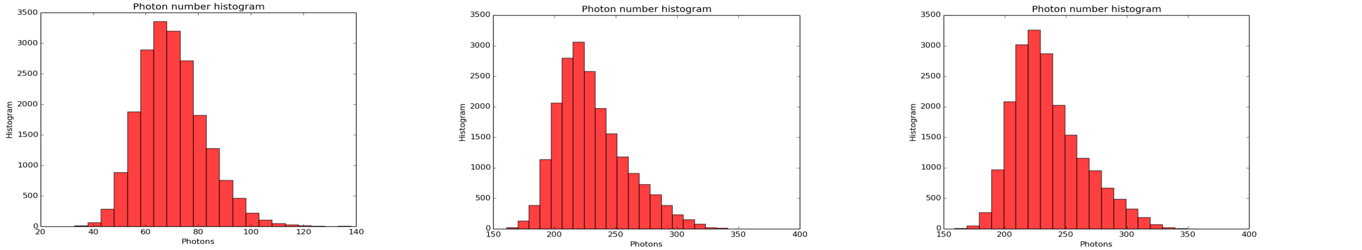
sample molecule 2NIP

Atom	τ_{Auger}(fs)
C	10.7
N	7.1
O	4.9
S	1.3
Fe	2.0

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



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



CFG et al., IUCrJ **4** (2017) Yoon et al. Scientific Reports **6** 24791 (2016)

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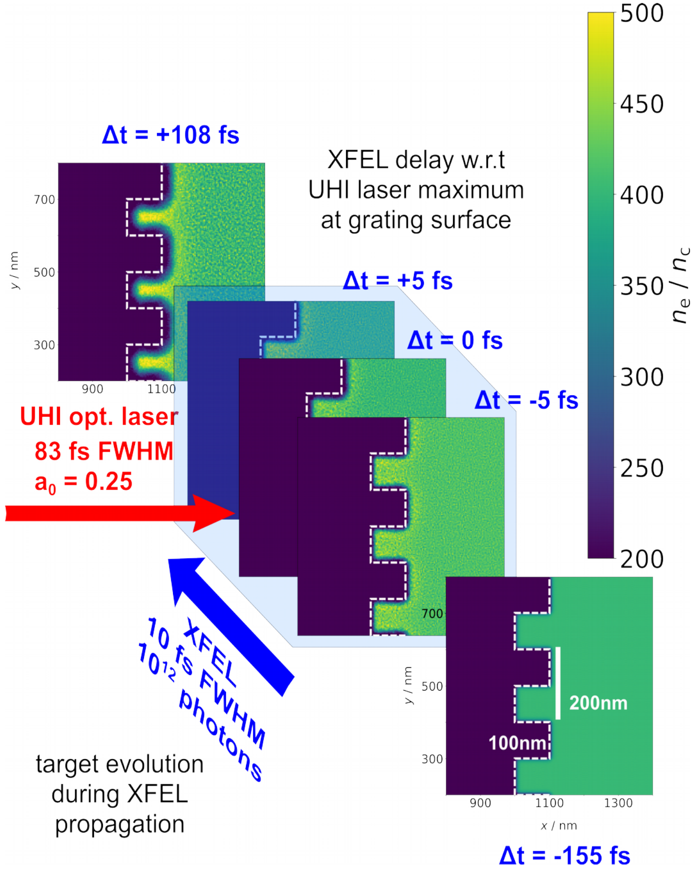
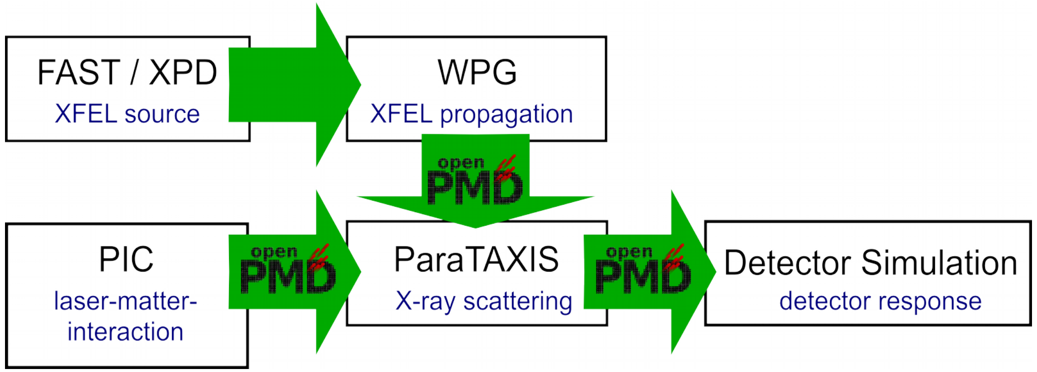
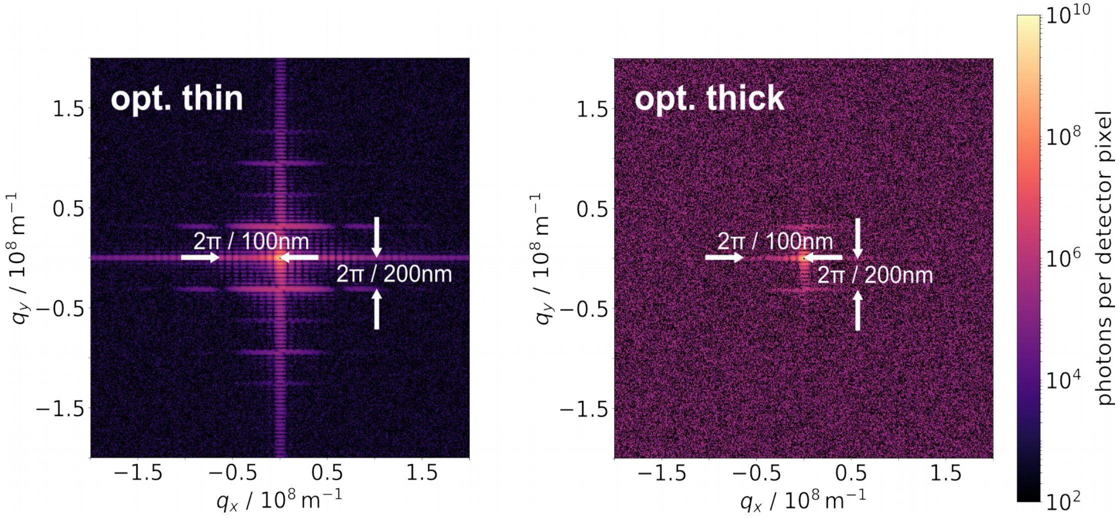
Monitoring the plasma evolution in structured targets







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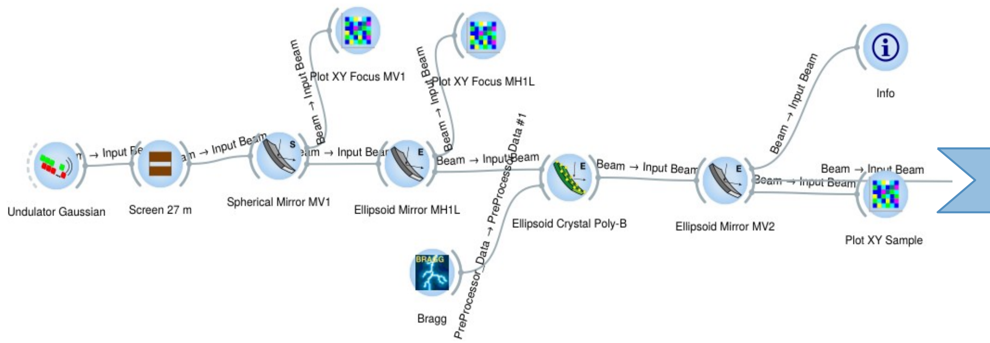
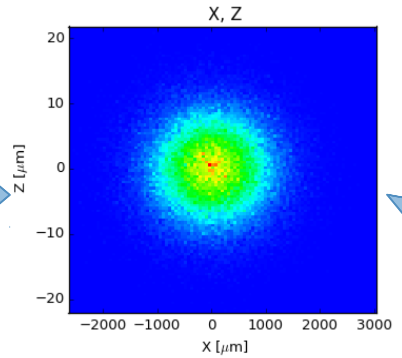
Simulation of long-pulse optical laser pump x-ray probe experiments

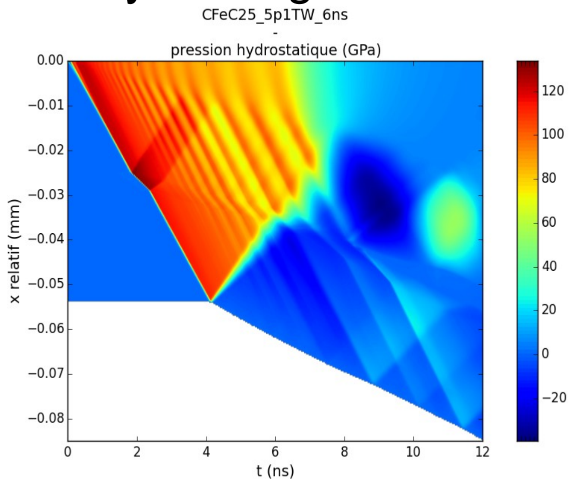
Synchrotron beam propagation (Oasys)



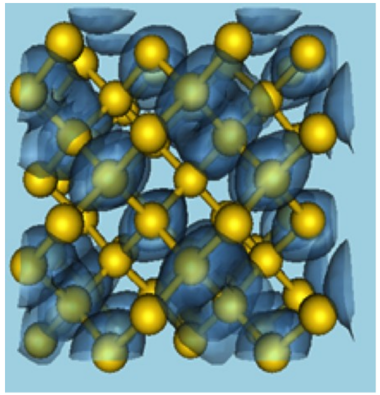
Beam profile at target position

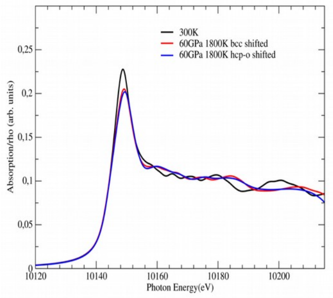


Rad-hydro target simulation



Electronic structure & response





XAFS signal (FEFF)

ESRF

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Summary

- PaNOSC will build cloud services of start-to-end simulations and data analysis for the large photon and neutron research infrastructures in Europe

- As a part of PaNOSC, SIMEX platform allows start-to-end simulations of complex photon experiments to help:
  - Optimize experiential parameters
  - Assess feasibility of proposed experiments (users, operators, reviewers)
  - Educate students, new members of group
  - Analyze experimental data

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Outlook

- SIMEX, as a part of cloud service ViNYL, will start with serving for SPB/SFX instrument in this project
- Keep SIMEX extensible, especially for high performance computing required by the researches of high energy density, mater in extreme conditions and other complex systems
- Define harmonized data format standards (openPMD) for simulation modules across ViNYL, and be compatible to to experimental data formats

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The openPMD standard for particle-mesh data

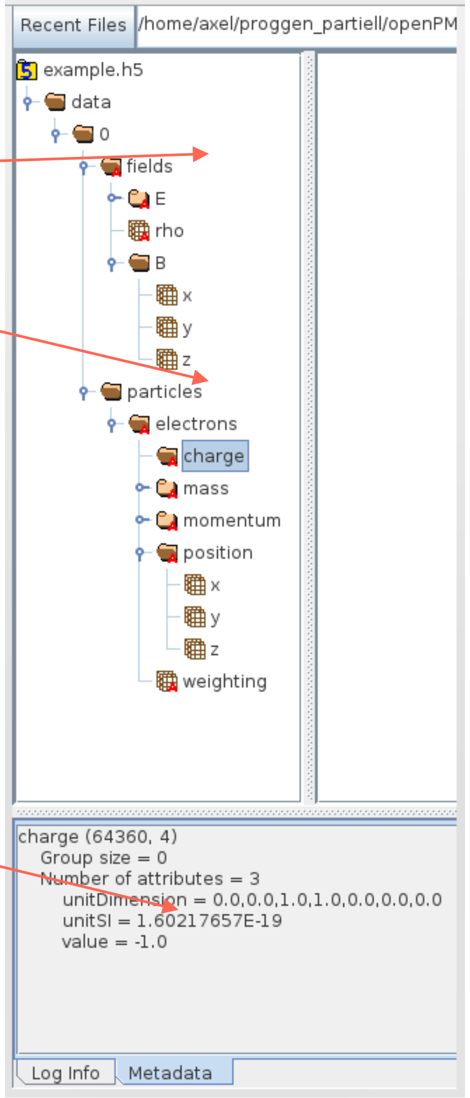
http://www.openpmd.org

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

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

- Transparent support for physical units through standardized unit conversion scheme

- Application specific domain extensions:
  - PIC, wavefronts
  - Rad-Hydro
  - MD
  - QMD



[A. Huebl & M. Bussman, HZDR]

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openPMD Eco-System

github.com/openPMD/openPMD-projects

openPMD standard (1.0.0, 1.0.1, 1.1.0)
the underlying file markup and definition
A Huebl et al., doi: 10.5281/zenodo.33624

base standard
general description

extensions
domain-specific
e.g. ED-PIC, SpeciesType, BeamPhysics

native data tools
HDF5, ADIOS, NetCDF, ...
e.g. h5ls, h5repack, h5dump, bpdump

writers & converters
simulations, frameworks, measurements
e.g. PIConGPU, SIMEX_Platform

HDF Compass
HDF5 & ADIOS file explorer
open and explore file trees

readers
coupled simulations, post-processing frameworks, ...
e.g. SIMEX_Platform, VisIt, yt-project, openPMD-viewer

openPMD-updater
update to new standard
edit in- or new file

data repositories
exchange and long-time archival
e.g. Zenodo, RODARE (HZDR)

[A. Huebl & M. Bussman, HZDR]

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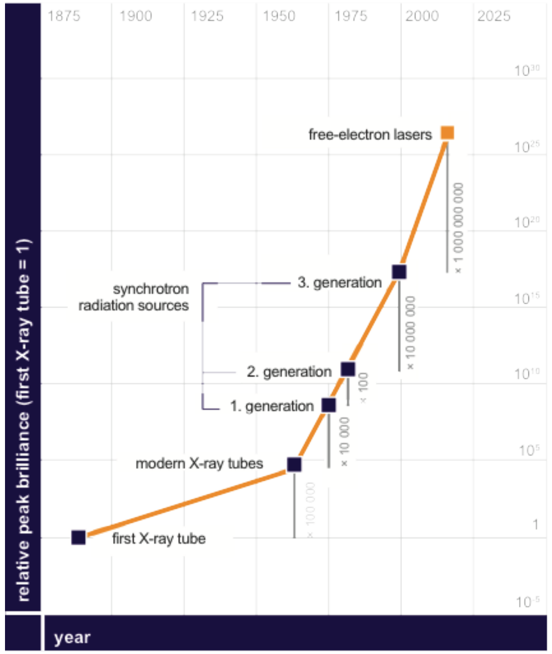
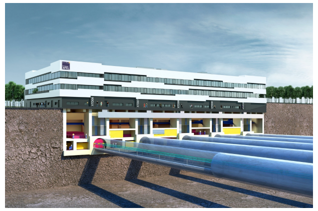
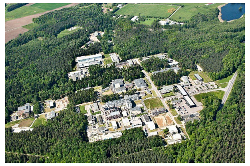


- Photon facilities combine x-ray and optical laser sources to make an up-to-date research infrastructure:
  - Pump-probe techniques
  - Creation of extreme states of matter
  - Sample control and *in situ* characterization
  - fs – ns temporal scale
  - Å – nm spatial scale

- Ultra-short & ultra-intense pulses of x-rays and optical laser light
  - Common technological challenges:
    - ► Pulse control and characterization
    - ► Data acquisition
    - ► Sample/target delivery
    - ► Theory and simulations of complex experiments



EuXFEL



HZDR

ELI

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