SIMEX – a platform to perform start-to-end simulations of XFEL experiments

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LEAPS Integrated Platform Workshop
May 11th, 2021

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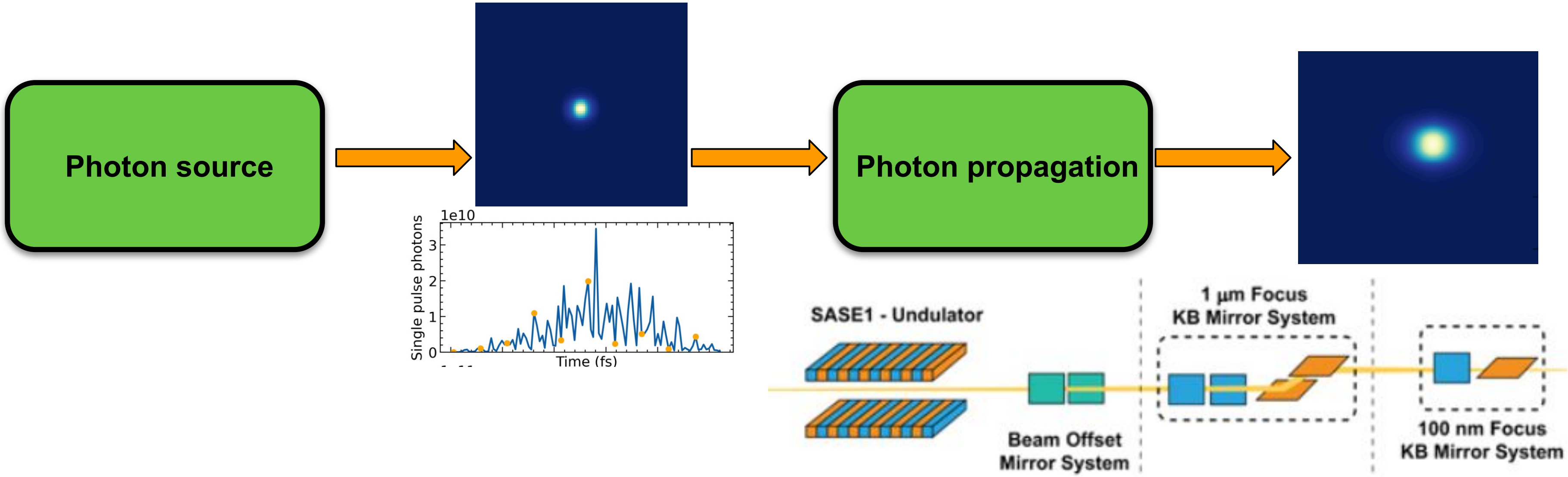
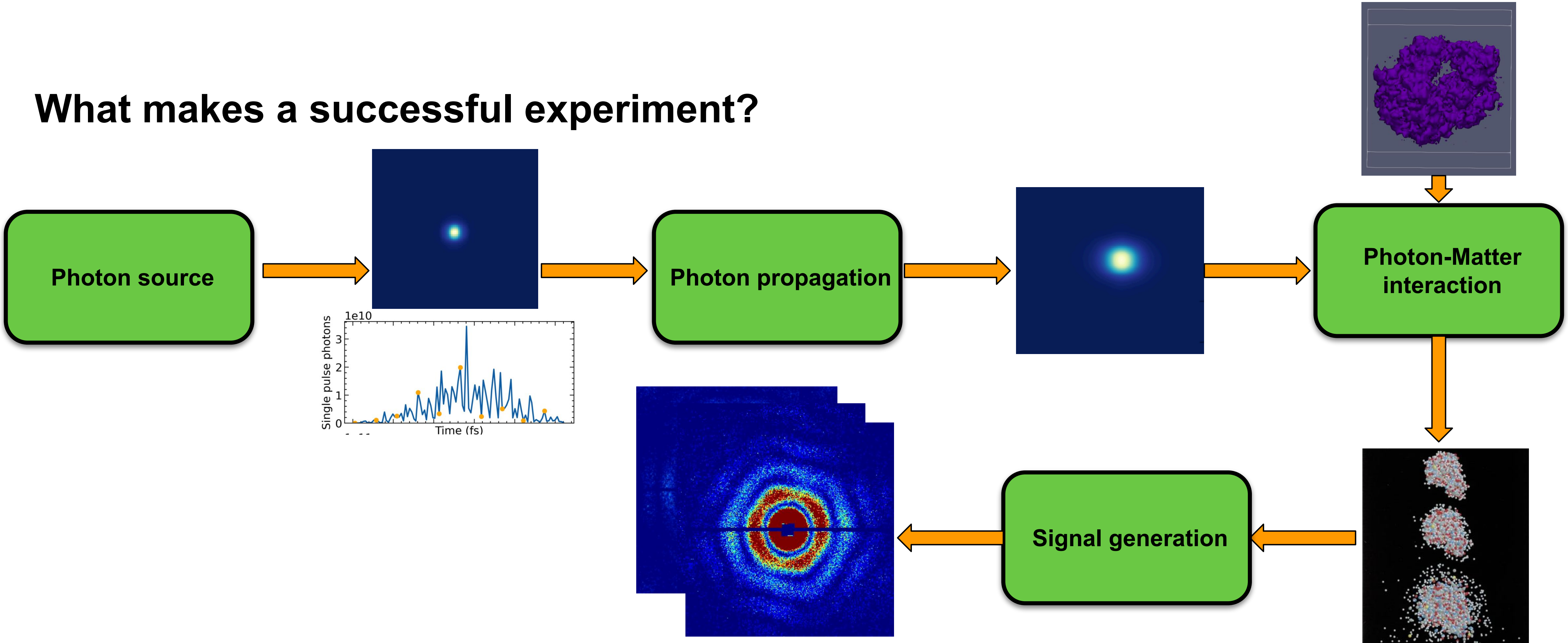
What makes a successful experiment?

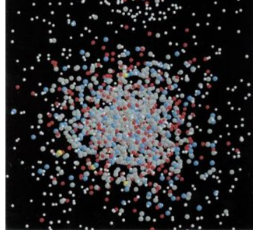


- How should the accelerator be configured to produce the “best” pulses?
- How do FEL components and configurations degrade, or enhance, experimental results?
  - e.g. Heat load influence on asymmetric crystal optics
- How do real pulses (e.g. SASE pulses with fluctuations), instead of idealised pulses, propagating through the instrument interact with the optics?

Mills, G., Bean, R. & Mancuso, A. P. Applied Sciences 10, 3642 (2020).

What makes a successful experiment?





- What will happen during the interaction?
- Does that influence what can be measured on the detector?

Neutze, R., Wouts, R., van der Spoel, D., Weckert, E. & Hajdu, Nature 406, 752–757 (2000).
Yoon, C. H. et al. Scientific Reports 6, 24791 (2016).
Fortmann-Grote, C. et al. IUCrJ 4, 560–568 (2017).

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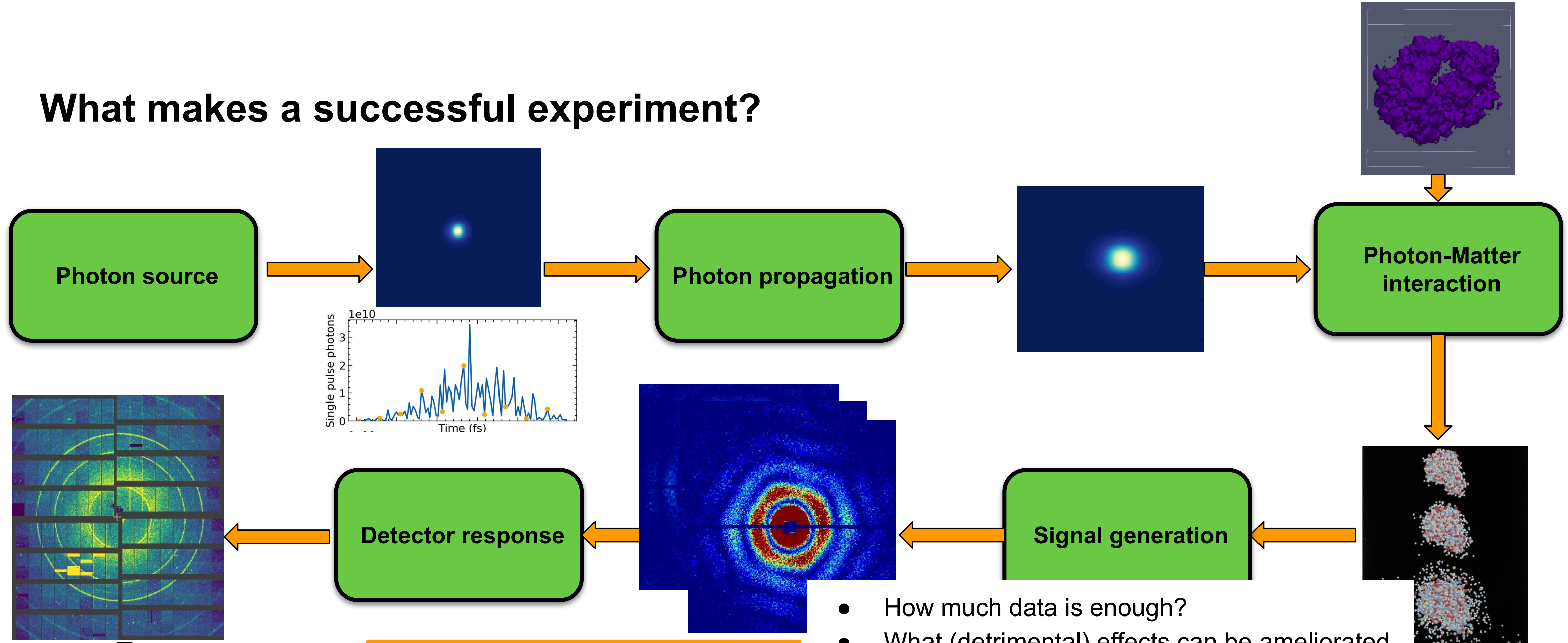

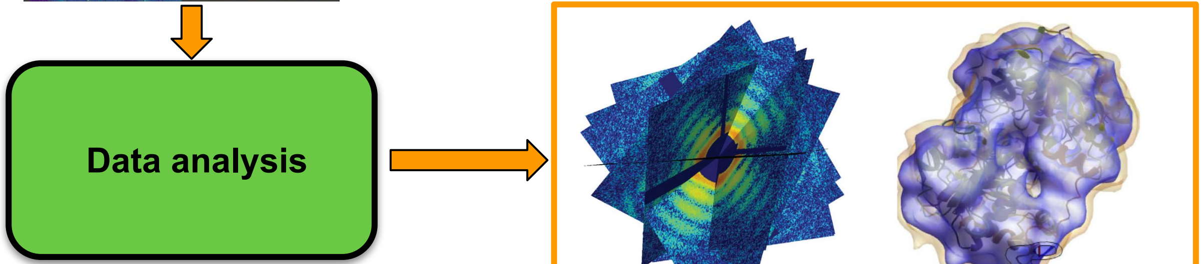

- How much data is enough?
- What (detrimental) effects can be ameliorated by simply collecting more data?
- What's the smallest particle size practically visible in a single particle imaging experiment

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Ekeberg, T. et al. Physical review letters 114, 098102 (2015).
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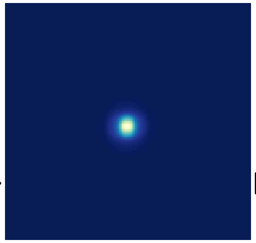
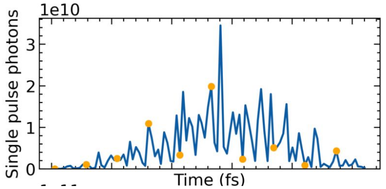
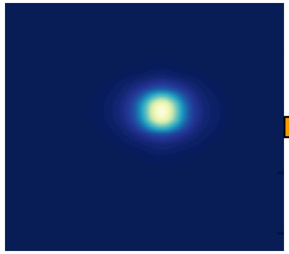
What makes a successful experiment?

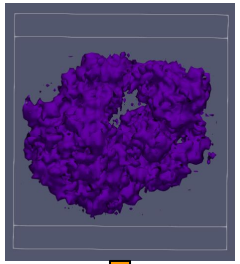
Photon source



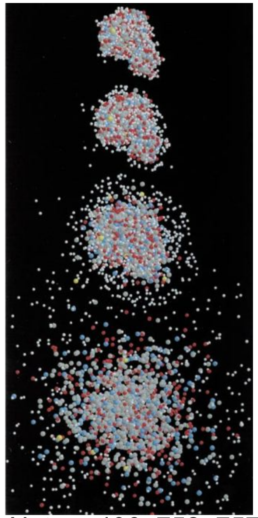


Photon propagation



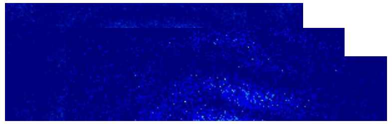


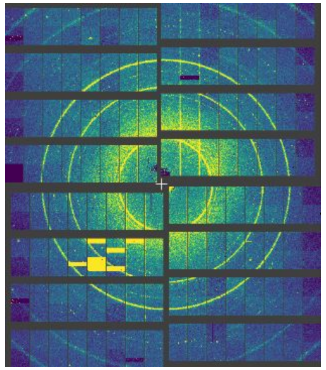
Photon-Matter interaction



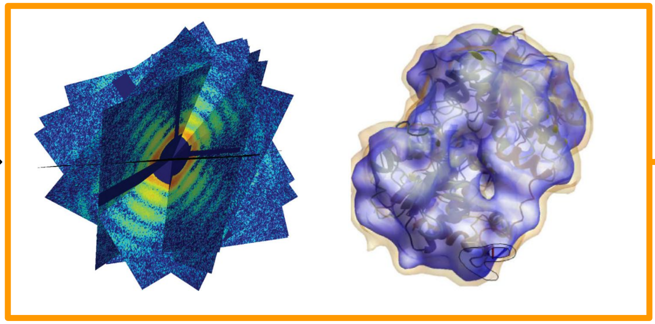
nal generation

- How should the accelerator be configured to produce the “best” pulses?
- What’s the definition of the “best” pulses?





Data analysis



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What parameters can be understood/optimized through Start-to-end simulations

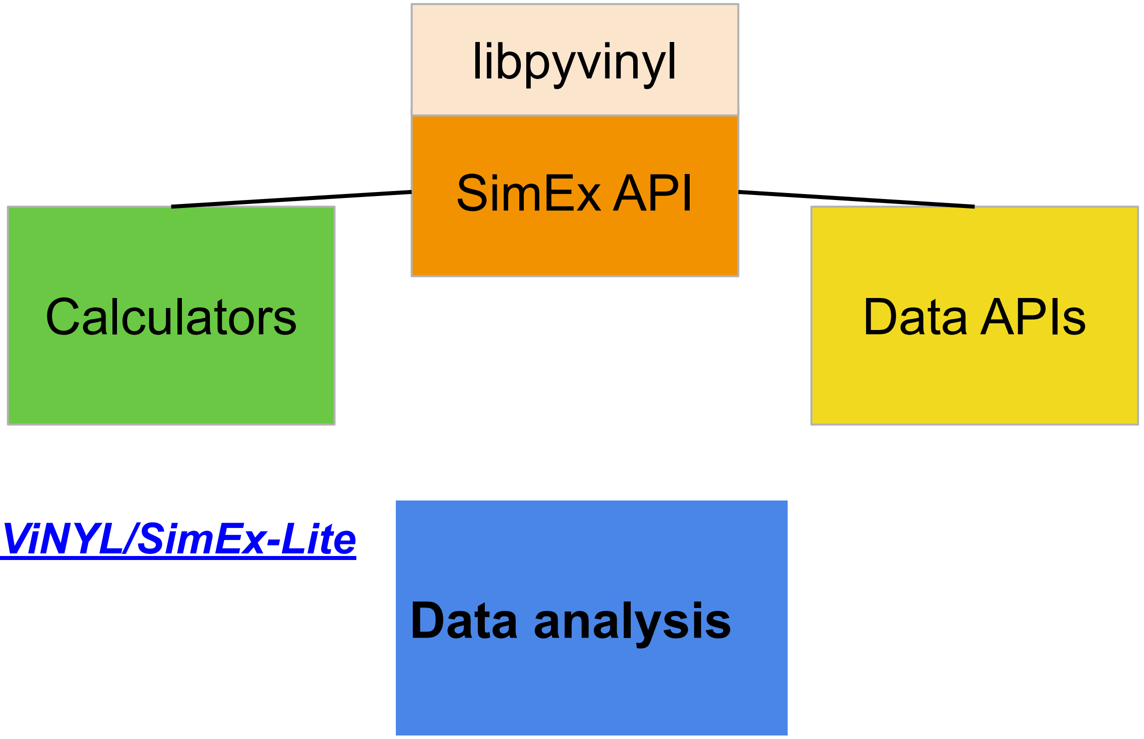
- Photon source
  - Pulse duration, repetition rate
  - Pulse (temporal and spatial) profile shape
  - Pulse energy
  - Beam wavelength
- Beamline optics
  - Optics (mirror, lens, monochromator, ...) parameters (profile, distance)
  - Beam wavelength
- Sample
  - Sample environment (water layer, ...)
- Detector
  - Geometry (detector distance)
- Data analysis methodology
  - Validate data analysis methodology
  - Estimate required amount of data/resolution limitation/…

And more…

almost unlimited possibility

SIMEX platform

- SimEx: a python library for start-to-end simulations of complex photon science experiments
  - Calculators: APIs for advanced simulation codes
    - ► Generate input parameters for calculator backengines
    - ► **Start & monitor backengine execution**
  - Data APIs provide data to the calculators based on open metadata standards and hierarchical file formats (HDF5)



- Photon source
- Photon propagation
- Photon-matter interaction
- Signal generation
- Detector

- Wavefront **OpenPMD** extension
- Molecular Dynamics **OpenPMD** extension
- **NeXus format**

SimEx-Lite:
https://github.com/PaNOSC-ViNYL/SimEx-Lite
Under development

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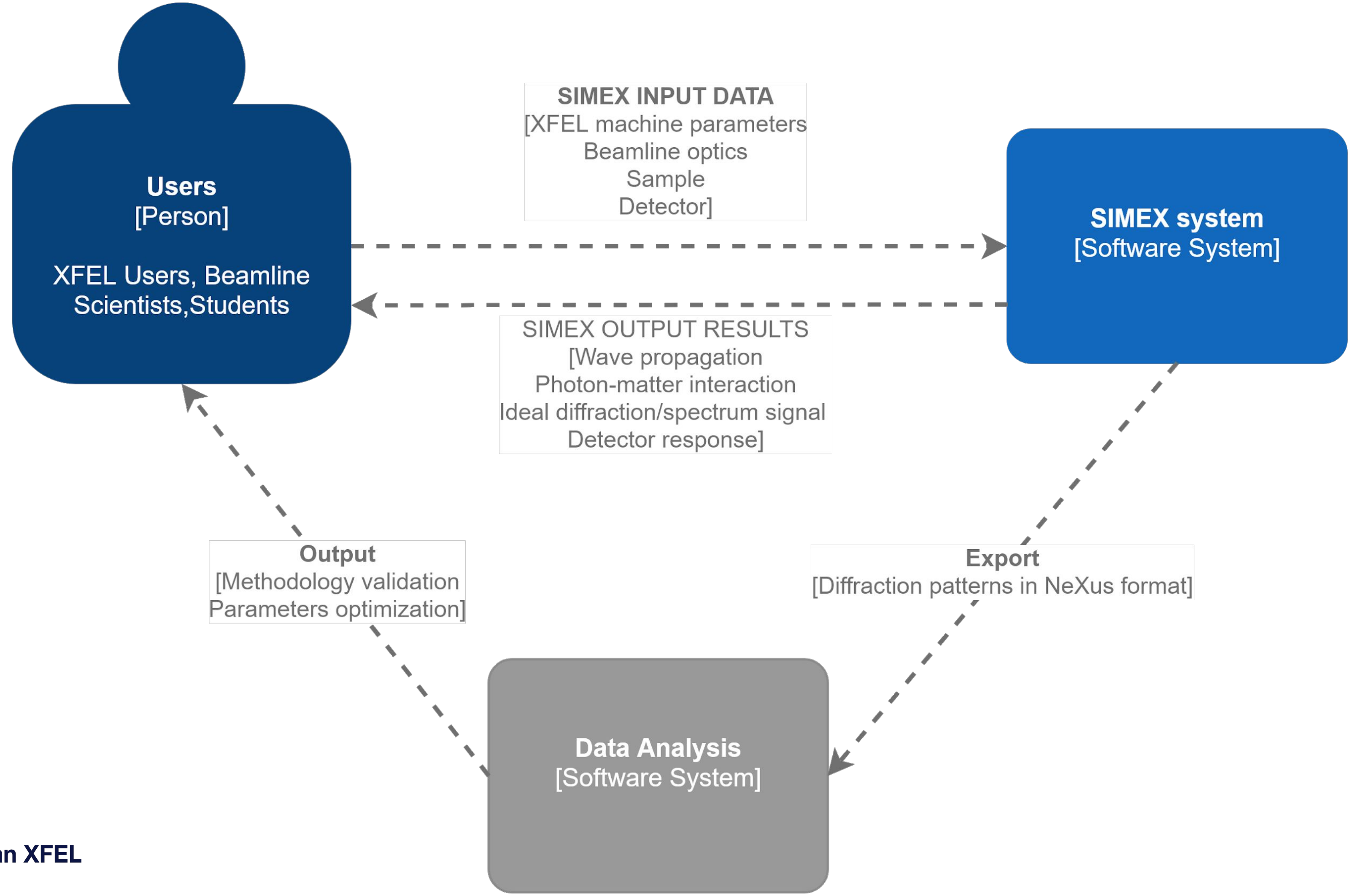
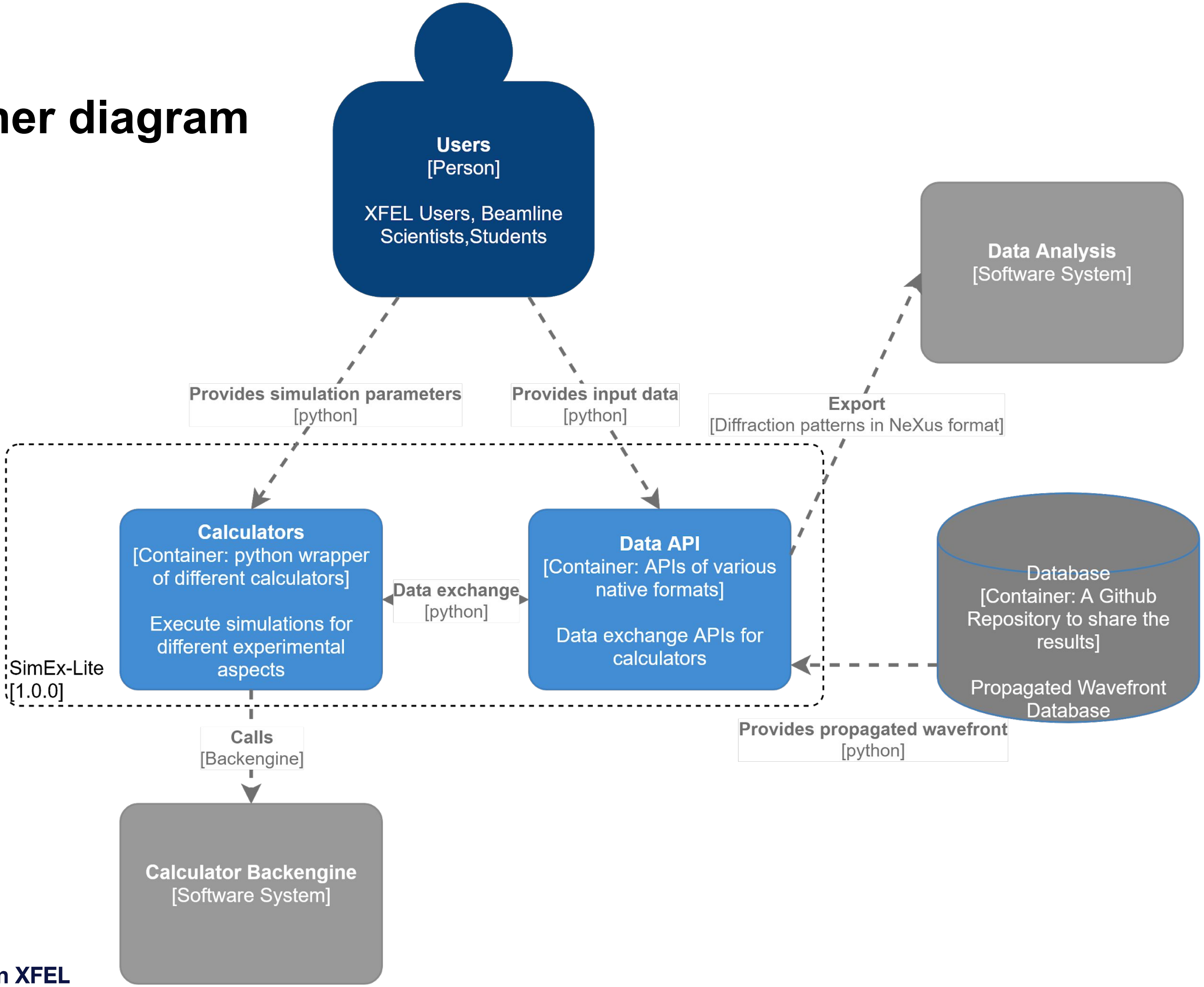
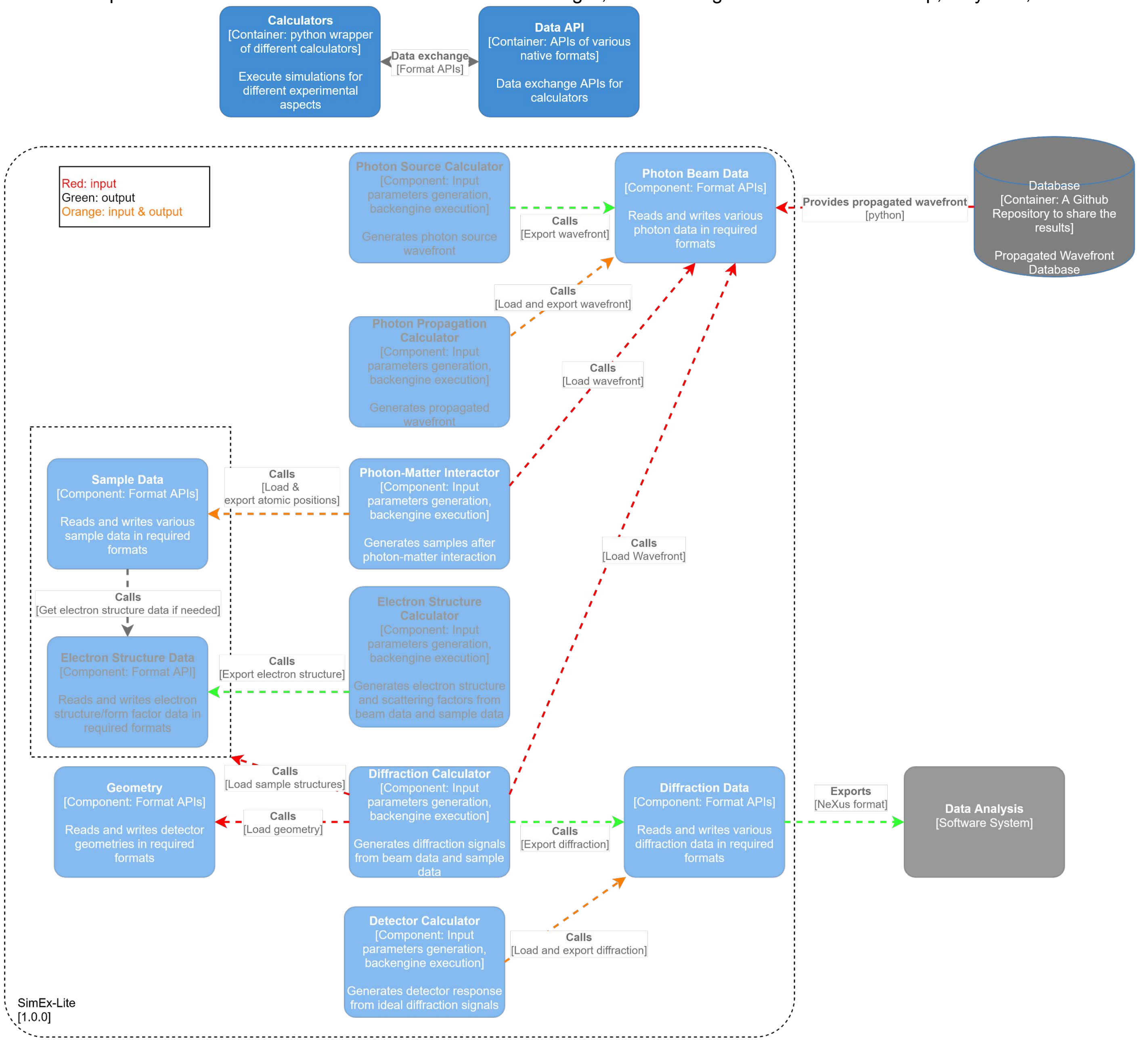
SIMEX system context diagram



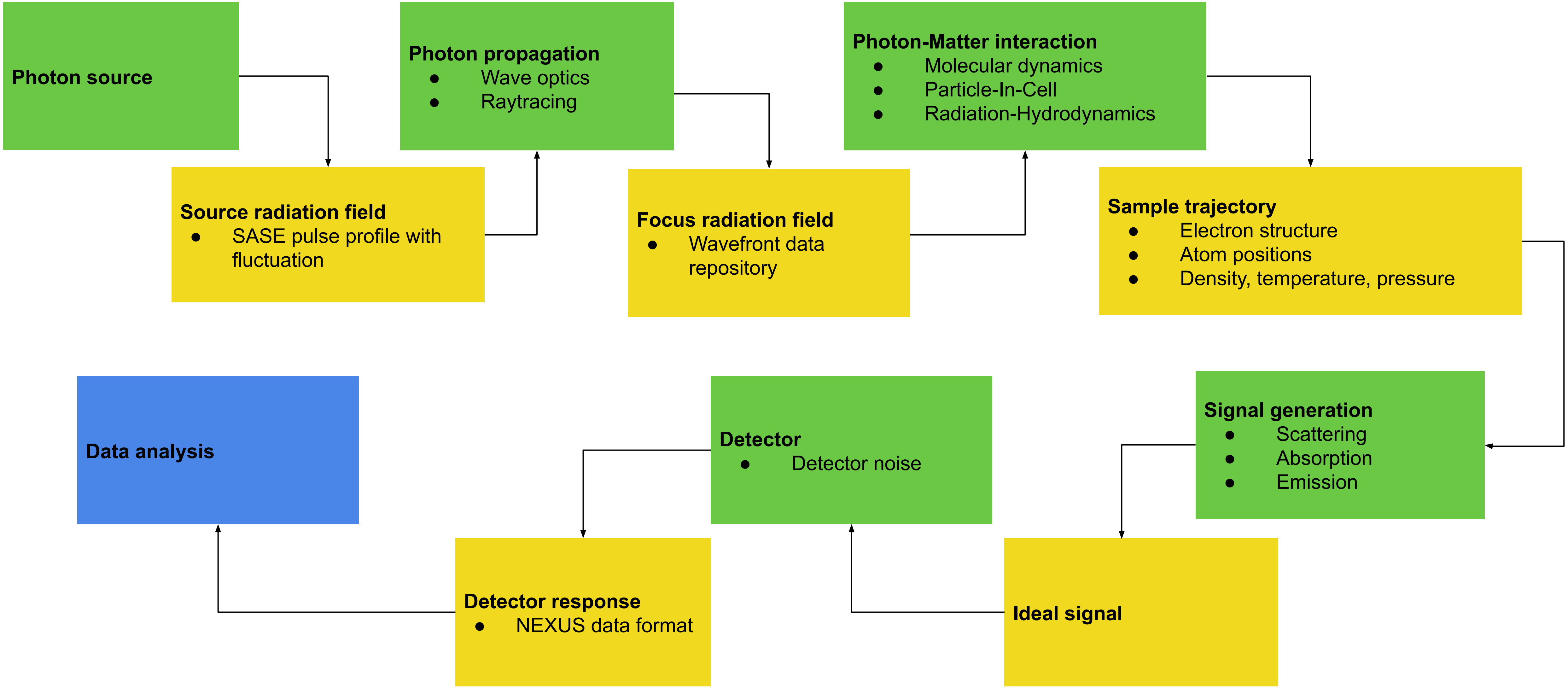
SIMEX container diagram



Component diagram



Workflow


Photon source
Source radiation field
SASE pulse profile with fluctuation
Photon propagation
Wave optics
Raytracing
Focus radiation field
Wavefront data repository
Photon-Matter interaction
Molecular dynamics
Particle-In-Cell
Radiation-Hydrodynamics
Sample trajectory
Electron structure
Atom positions
Density, temperature, pressure
Signal generation
Scattering
Absorption
Emission
Ideal signal
Detector
Detector noise
Detector response
NEXUS data format
Data analysis

List of calculators

Module	Simulation type	Code	Collaborators
X-ray source	FEL simulation	**FAST-XPD**	**Yurkov, Schneidmiller, Manetti, Samoylova**
		GENESIS in OCELOT framework	S. Reiche / G. Geloni et al.
Propagation	**Coherent wavefront propagation**	**WPG/SRW [Data repository in preparation]**	**L. Samoylova, A. Buzmakov, O. Chubar**
X-ray photon matter interaction	Atoms, molecules, clusters	**XMDYN & XATOM**	**Z. Jurek et al. (CFEL)**
		GROMACS	**I. Dawod et al. (U Uppsala)**
		HF/LDA	*H. Quiney et al. (U Melbourne)*
Optical photon matter interaction	1D Rad-Hydro	Esther	Colombier et al. (CEA)
	3D PIC	PiConGPU	M. Bussmann et al. (HZDR)
Signal generation	**Molecule, cluster scattering**	**SingFEL/skopi**	**C. H. Yoon (LCLS)**
	Plasma SAXS	paraTAXIS	T. Kluge et al. (HZDR)
	Plasma Compton/Thomson	XRTS	G. Gregori, C. Fortmann-Grote
	Crystal diffraction	**CrystlFEL/pattern_sim**	**T. White et al. (CFEL)**
	Diffraction (large atomic system)	**GAPD**	**J. C. E, S. N. Luo et al.**
	EXAFS	FEFF8L	J. J. Rehr et al. (U Washington)
Detector simulation	2D Pixel detectors	X-CSIT, Karabo	T. Rüter et al. (EuXFEL)

Developed actively and will be included in Lite; Implemented before, maintain on demand; *Planned for future interfacing*

Further work

- Real detector behaviours
  - If the detector performance is not good enough, even if the sample and other instrumentation behaves well, the experiment still may not succeed.
- Simulation result - XFEL source/beamline parameter feedback loop
  - Optimize the XFEL source/beamline parameters based on detector signal (e.g. diffraction pattern, spectrum) or reconstructed data (e.g. 3D orientation and phase reconstruction) quality.
- AI training cases
  - Estimate XFEL spectrum from machine parameters with AI algorithm
- Single particle imaging methodology understanding/optimization
  - Ascertain the smallest particle size practically visible in a single particle imaging experiment
- … and more

Challenges

- More user friendly code developments
  - Easy installation
  - Comprehensive documentations and examples
  - Best practice for high performance computing
  - Accessibility to different users
  - Encouraging more people to get involved
- User expertise
  - Every step of start-to-end simulation requires corresponding knowledge to understand the assumption and limitation of the simulation method to be used
  - Simulation database could be a solution
  - Machine learning use case

Acknowledgements

European XFEL: **Adrian Mancuso**, **Carsten Fortmann-Grote**, **Michal Stransky**, **Chan Kim**, Thomas Kluyver, Yoonhee Kim, Raphaël de Wijn, Marcin Sikorski, Johan Bielecki, Henry Kirkwood, Liuba Samoylova, Alexey Buzmakov, **Juncheng E**

DESY, CFEL Science: **Beata Ziaja-Motyka, Zoltan Jurek**

Uppsala Universitet: **Ibrahim Dawod**, Carl Caleman, Nicusor Timneanu

NUS National University of Singapore: Shen Zhou, Duane Loh

EUCALL: The European Cluster of Advanced Laser Light Sources (2015-2018)

SLAC: Chuck Yoon, Christopher Mayes, Jacek Krzywinski, Hugo Slepicka, Paul Fuoss

Brookhaven National Laboratory: Oleg Chubar, Maksim Raktin

Berkeley Lab: Axel Huebl

panosc photon and neutron open science cloud: Aljosa Hafner (CERIC-ERIC), Mads Bertelsen (ESS), Mousumi Upadhyay Kahaly , Zsolt Lecz (ELI-HU), Shervin Nourbakhsh (ILL), Manuel Sanchez del Rio (ESRF)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 654220 and 823852

Links & References

Links

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- SimEx: https://github.com/PaNOSC-ViNYL/SimEx
- SimEx-Lite: https://github.com/PaNOSC-ViNYL/SimEx-Lite
- SimEx Documentation: https://simex.readthedocs.io/en/latest/
- SimEx Jupyter-notebooks: https://github.com/PaNOSC-ViNYL/SimEx-notebooks
- openPMD: https://github.com/openPMD
- NeXus: https://www.nexusformat.org/
- PANOSC-ViNYL : https://github.com/PaNOSC-ViNYL/ViNYL-project

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- J. C. E et al., in preparation