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

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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?

What makes a successful experiment?

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

What makes a successful experiment?

1. Photon source
2. Photon propagation
3. Photon-Matter interaction
4. Signal generation
5. Detector response
6. Data analysis

- 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?

What makes a successful experiment?

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

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)

**SimEx-Lite:**
[https://github.com/PaNOSC-ViNYL/SimEx-Lite](https://github.com/PaNOSC-ViNYL/SimEx-Lite)
Under development
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- Photon source
- Photon propagation
- Photon-matter interaction
- Signal generation
- Detector

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

Data APIs

Data analysis
SIMEX system context diagram
SIMEX – a platform to perform start-to-end simulations of XFEL experiments

SIMEX container diagram
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Component diagram
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**Workflow**

**Photon source**
- Photon propagation
  - Wave optics
  - Raytracing

**Photon-Matter interaction**
- Photon-Matter interaction
  - Molecular dynamics
  - Particle-In-Cell
  - Radiation-Hydrodynamics

**Source radiation field**
- SASE pulse profile with fluctuation

**Focus radiation field**
- Wavefront data repository

**Sample trajectory**
- Electron structure
- Atom positions
- Density, temperature, pressure

**Data analysis**

**Detector response**
- NEXUS data format

**Detector**
- Detector noise

**Signal generation**
- Scattering
- Absorption
- Emission

**Ideal signal**
## List of calculators

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<td>Plasma Compton/Thomson</td>
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<td>G. Gregori, C. Fortmann-Grote</td>
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<td>J. J. Rehr et al. (U Washington)</td>
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<td>2D Pixel detectors</td>
<td>X-CSIT, Karabo</td>
<td>T. Rüter et al. (EuXFEL)</td>
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</table>

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
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Links & References

Links

- 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

References

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- C. Fortmann-Grote et al., IUCrJ 4, 560–568 (2017)
- C. Fortmann-Grote et al., in Advances in Computational Methods for X-Ray Optics IV vol. 10388 103880M. doi: 10.1117/12.2275274
- J. C. E et al., in preparation