A proposal for a user-friendly modular framework for the simulation of x-ray experiments

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Abstract. As experimental concept and execution become increasingly complex across the spectrum of user-driven light sources, data analysis becomes more complicated and the urgency of completing an experiment on the first attempt grows. It has become apparent that simulation of the expected signal from such experiments can increase the likelihood of success of a particular experiment and the efficiency of a facility as a whole. Here, we propose a modular approach to the simulation problem, which will build on existing expertise and software. Additionally, we are working to support the simulation of partially coherent fields where the photon degeneracy parameter is much larger than unity.

1. Why invest in a new framework?
In a natural evolution of the x-ray user facilities and the communities they serve, state-of-the-art experiments increasingly rely on the detailed nature of the x-ray field interacting with the sample, whether this be related to the extremely large coherence volumes of current generation sources or the time structure of the probe in pump and probe experiments. Much of the optimization of these experiments is done “on the fly” during the allocated experiment time and is therefore not representative of the most efficient use of resources on the part of the facilities or their users. We believe that the excitement surrounding the rapid advances, especially in the spectral brightness and time structure of x-ray sources, and the increasing expertise of the user community can now be harnessed to provide a valuable toolset for simulating x-ray experiments and motivating even more exciting advances in sources (We note that projects similar to the one described here have been presented at previous international SRI meetings, c.f., the talk by Mancuso during Session P of the 2012 meeting).

Many tools already exist for the simulation of the output of a particular beamline at a given source (SHADOW)[1] and Synchrotron Radiation Workshop (SRW)[2] are excellent examples of these tools.; however, in most cases these are readily usable only by experienced beamline personnel and, in our experience, the models are rarely up-to-date because of the rapid advances that typify the progress of current x-ray sources. In this paper, we propose to develop a framework that overlays these existing tools and provides an enhanced and flexible expert and end-user experience. As the project progresses, we anticipate the expansion of the framework to include the simulation of probe-sample interactions and mock data analysis, which will provide a “one-stop solution” for designing and optimizing x-ray experiments.

2. Details of the proposal
Arguably the most important part of the nascent framework is the basic structure of the user interface and the parameterization of the x-ray field. We believe that this process must involve a broad cross section of the community and continue to seek input from interested parties. We propose to discretize the simulation process by defining a series of discrete events that represent the propagation of a data object through vacuum or matter. For a schematic diagram, see figure 1.
2.1. The data object

Our data object is the electric field. Provisions are made to store the following in a Cartesian space:

1. the complex field magnitude in the plane perpendicular to the propagation direction (We define this as the z-axis.), which is parallel to the Poynting vector at the source (We define this as the lab frame.) and subsequently determined by the field’s interaction with matter;
2. the components of the field’s polarization;
3. the energy spectrum of the field, defined around the mean frequency by a variable number of slices at user-defined resolution;
4. the instantaneous time structure of the field, beginning at the “front” of the field at some time-zero and extending backward along the time axis;
5. inclusion of harmonic content, with the field’s properties understood to scale as a multiple of the spectrum;
6. the mean photon energy;
7. the absolute energy that should be obtained by integrating the intensity over time, space, and frequency;
8. the bounds on each of the field’s variables(metadata);
9. the increment of each of the field’s variables(metadata);
10. the position in the 3D lab frame(metadata);
11. the integrated optical path length(metadata) and total time of flight; and
12. an Euler matrix describing the orientation of the current reference frame with respect to the lab frame(metadata).

2.2. The data structure

The data structure contains:

1. a multidimensional array with internal structure like so:
   
   \[
   \begin{array}{|c|c|}
   \hline
   \text{hor., vert. polarization} & \text{time} \\
   \hline
   \text{spectrum} & \text{horizontal, vertical position} \\
   \hline
   \text{real, imag. magnitude} & \text{real, imag. magnitude} \\
   \hline
   \end{array}
   \]
   
2. scalars representing the bounds and increments for the time, spectrum, and transverse position;
3. scalars representing mean photon energy, absolute integrated energy, lab frame z-position, and optical path length;
4. a vector indicating the pointing of the local frame’s propagation direction relative to the lab frame;
5. strings containing unit information for the physical properties; and the identifier of the last module to handle the data object.

The object and its metadata are presented to a *module*—a method that manipulates the data object, e.g., propagation or a focusing mirror—and returns an updated data object.

Figure 1. A modular, event-based approach to simulating an x-ray experiment from the source to the detector provides users the opportunity to use prebuilt models for each interaction or to provide their own, depending on the specific requirements of the experiment.
2.3. Modules and events
Every event during the propagation of the simulated field is handled by a module. Every module accepts as input the data structure and metadata specific to that module, for example, a module that simulates the focused beam due to a pair of Kirkpatrick-Baez mirrors might take as metadata the x-ray incidence angle. Additionally, the module might include a detailed physical description of the field’s interaction with the mirrors or a simple reflectivity curve.

Free space propagation is also treated in a module, where one can choose to propagate the field as a coherent object or take into account its detailed coherence properties. We are currently evaluating a coherent mode decomposition approach for the propagation of partially coherent fields[3]. For simulation of the field from the source to the sample location, we propose to remain in the paraxial approximation during free space propagation.

As the project matures, we anticipate the contribution of modules, especially those dealing with high field strengths or time dependent interactions, from the general user community.

2.4. The storage format
One HDF5[4] file is saved after the return of each module. The goal for the file format is two-fold: to record the information contained in the data structure and to record the “history” of the field. The file format has the following structure:

```
/event0
  /<data object>
  /<data object parameter 1>
  .
  .
  /<data object parameter N=12>
  /origination information (source identifier)
  /author/time stamp
/event1
  /data object
  ...
  /origination information (module identifier)
  /author/time stamp
  .
  .
```

The /event<> identifiers are either full data structures or symbolic links to groups within other HDF5 files.

2.5. Underlying tools
We believe that it is of vital importance to ensure that this framework is widely and freely available. To facilitate this goal and maintain a reasonable scope of work, we propose to embrace open source technology. In particular, we believe that the Python programming language[5] is an excellent foundation for the framework:

i. it is widely and freely available;
ii. modules written in nearly any programming language can be incorporated into the framework through the use of “wrappers;” and
iii. it natively supports “command line” input and is readily extended to include graphical user interfaces that are essentially platform independent.
3. Summary

We have briefly out-lined our current draft specification of a framework that we believe will enhance the user experience, planning activities, and efficiency of operation of x-ray facilities. We are eager to engage all invested parties in the development and realization of this project, while adhering to goals of open access and user contribution to the framework.

Appendix A. Acknowledgements
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References
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[4] Folk M, Heber G, Kozoil Q, Pourmal E, and Robinson D 2011 AD ’11 Proceedings of the EDBT/ICDT 2011 Workshop on Array Databases 36.
[5] See http://www.python.org for more information on the Python programming language.