SRN 36_5 guest editorial

The design of x-ray optical systems is very different from that of conventional optical systems, whether it be for the peculiarities of synchrotron radiation or the grazing incidence operation of most x-ray optical components. Specific simulation tools are thus required to ensure that designs work as expected, and there is now a vibrant landscape of open-source, freely available software that can be used to that end, and explore new design concepts.

This is particularly true in the context of 4th generation light sources, including diffraction-limited storage rings and free electron lasers that are being built and commissioned worldwide. These facilities provide x-ray beams that are almost fully coherent and require optical components that can preserve this coherence, pushing the limits of manufacturing capabilities. A fraction of a nanometer difference in the figure error tolerance of a mirror can double the cost of the optics, thus allocating fewer resources for other components. Simulation tools help ensure that tolerances reach an optimal tradeoff.

Beamline simulation tools can be separated into two main categories: raytracing, where the light is considered incoherent and freely bouncing off mirrors, and wavefront propagation, where light is considered coherent and can interfere with itself. These two approaches are equally useful but conceptually incompatible due to the wave/particle duality of light; there are many efforts to create hybrid descriptions and deal with partially coherent beams. In addition, new tools have emerged over the past few years, providing a graphical user interface for their users, making them more accessible and helping design teams to collaborate, and move from specification requirements to optical design to mechanical implementation more smoothly.

In this issue, Manuel Sanchez del Rio from the European Synchrotron Radiation Facility and Luca Rebuffi from the Advanced Light Source provide a historical perspective on the development of Shadow, one of the original raytracing simulation software, and on Oasys, a more recent effort to bring various simulation software together using a graphical user interface.
Takasi Tanaka from SPRING-8 describes the latest developments available in Spectra, a simulation software dedicated to synchrotron radiation simulation, with an emphasis on the effects of coherence that are increasingly important when dealing with 4th generation light sources. Oleg Chubar and colleagues from the National Synchrotron Light Source (II) detail how the Synchrotron Radiation Workshop (SRW) wavefront propagation software allows for the simulation of the source, the beamline components, and the experiments.
Konstantin Klementiev and Roman Chernikov from MAX-IV explain how XRayTrace, also known as xrt, blends together raytracing and wavefront propagation, to help study new states of light that will be accessible to new light sources.
John Sutter and colleagues from the Diamond Light Source discuss how analytical derivations can be combined with all these tools to help the design of state-of-the-art beamlines.
Finally, Ken Goldberg from the Advanced Light Source reports on efforts to gather the community of beamline designers together, after the pandemic grounded these interactions to a halt.

With recent advances in machine learning, we are now at a time where simulations can interact with experiments, through the creation of digital twins – accurate virtual representations of a beamline. These can be used to help scientists better understand the performance of their beamlines while they're using them, and to train models for automated alignment routines. Diffraction-limited beamlines will require such fly-by-wire operation, and the light source users community will indeed be able to enjoy x-rays limited by physics only – and their imagination.

We tremendously enjoyed collecting these pieces from colleagues worldwide, and we hope you'll enjoy reading them too!

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