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# ***Advances in Computational Methods for X-Ray Optics III***

**Manuel Sanchez del Rio  
Oleg Chubar**  
*Editors*

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## Introduction

This SPIE 9209 Conference, *Advances in Computational Methods for X-Ray Optics III*, comes three years after the second edition (SPIE 8141). It is our intention to organize this conference with three-year frequency—leaving time to witness the important developments in the field. 10 of the 28 oral presentations were invited. An interesting poster session opened the conference sessions with five more papers. Sessions were dedicated to Fundamentals and Facility Reports, Methods and Codes, Instruments and Beamlines, Crystal Optics, and High-Resolution Focusing Optics and Imaging. A satellite workshop on “Software for Modeling X-ray Sources, Optics and Scattering” completed and complemented the program of the conference with live demonstrations of software tools.

The numerous presentations demonstrated considerable progress in the field since the last conference: stimulated, to large extent, by the construction and start of operation of the new synchrotron and XFEL sources and the challenging upgrade of the existing ones. This evolution and in particular the continuously growing importance of the wave-optics simulations for the low-emittance synchrotrons and for x-ray FEL, was emphasized by Kwang-Je Kim in his opening talk. Other speakers from most important X-ray sources (Diamond Light Source, European XFEL, ESRF, LCLS, NSLS-II, MAX-IV, APS, Elettra) discussed the news from their facilities with examples of simulations for beamlines. The presentations showed that most new beamline simulations were modeled using well established software codes (SRW, SHADOW, PHASE, McXtrace) and in many cases the calculations used more than one code which stressed the adequacy and limitations of the different codes depending on the phenomena and radiation characteristics to study. Calculations of partially coherent emission and radiation propagation are extensively demanded for the new facilities, and SRW demonstrated its suitability for these simulations and is taken as a reference. Several new developments in SRW extended its range of applications to cover grazing incidence focusing mirrors, variable line spacing gratings and crystals. Merging wave-optics and ray-tracing into hybrid methods is another tendency that has been observed, and it opens the way to new tools that will permit to simulate experiments using simultaneously several codes. New developments for treating and analyzing scattering from mirror imperfections were presented. A crystal optics session covered a number of new developments and applications including high-resolution crystal systems, coherent imaging of photonic crystals, applications for plasma diagnostics, and imaging optics in laboratory sources.

Although most of the talks were related to synchrotron radiation sources (of third and fourth generation), a few presentations were dedicated to other x-ray sources (plasma physics, astrophysics). The last session on High-Resolution Focusing Optics and Imaging included experimental and modeling works for phase contrast imaging using laboratory sources. The Conference triggered a

rich exchange of information among different communities that share optical designs and methodological approaches for dealing with x-rays.

The workshop on "Software for Modeling X-ray Sources, Optics and Scattering" followed the talks and was well attended. The workshop was limited to short demonstrations of software updates, in three blocks related to McXtrace, SHADOW and SRW. E. B. Knudsen discussed last applications of McXtrace and showed a web-based interface. P. Sondhauss demonstrated MASH, a web-based environment to simulate beamlines powered by COMSOL and SHADOW. M. Sanchez del Rio briefly discussed the evolution of XOP, upgrading the current version to 2.4, and exploring a new version to be integrated into an Orange-based common tool. L. Rebuffi showed a modern and performant interface to SHADOW under Orange. In the last block dedicated to SRW, O. Chubar briefly presented the latest news, including the on-going development of the "virtual beamline" library targeting to facilitate commissioning of new beamlines and simulation of experiments, then D. Bruhwiler demonstrated the use of a web-IPython-based interface for SRW, and finally L. Samoylova presented the IPython environment built on top of SRW for the simulations at the European XFEL.

We are indebted to our co-chairs Carolyn MacDonald and Kawal Sawhney for their enthusiasm and help in the organization of this conference, and also to the members of the Program Committee for their invaluable assistance.

**Manuel Sanchez del Rio**  
**Oleg Chubar**