ESRF

Elettra Sincrotrone Trieste

Software for Optical Simulations

Workshop

Trieste,
3rd – 7th October 2016

KYMA

radiasoft

Rigaku

DECTRIS®

imagine optic

WYROWSKI PHOTONICS

STRUMENTI SCIENTIFICI CINEL® s.r.l.

Leading experts in optics for synchrotron and FEL radiation, side by side with authors and developers of state-of-the-art optical simulation software tools, showing their best usage with advanced uses cases.

Key Topics:

- Ray-Tracing: Soft and Hard X-ray SR-Beamlines
- Wavefront Propagation: SR and FEL Beamlines
- Optical Calculation Tools
- Industrial Applications

Invited Speakers:

Oleg Chubar (BNL)
Daniele Cocco (SLAC)
Carsten Fortmann-Grote (XFEL)
Ruben Reininger (ANL)
Liubov Samoylova (XFEL)
Rami Sankari (MAX IV)
Xianbo Shi (ANL)
Sergey Stepanov (ANL)

Local Organizing Committee:

Luca Rebuffi (Elettra)
Marco Zangrando (Elettra, IOM-CNR)
Manuel Sanchez del Rio (ESRF)

http://www.elettra.eu/Conferences/2016/SOS/

INDEX

INTRODUCTION

In the next few years, all the major synchrotron radiation facilities around the world will be upgrading to 4th generation Diffraction Limited Storage Rings (using multi-bend-achromat technology). Several Free Electron Lasers are ready-to-go or in phase of completion. These events represent a huge challenge for all the Optics physicists, responsible of the calculations needed to design and produce the new optical elements, able to deal with the revolutionary characteristics of the new photon beams.

Therefore, the target of the SOS (Software for Optical Simulations) workshop is to put together leading experts in optics for synchrotron and FEL radiation with authors and developers of state-of-the-art optical simulation software tools. The workshop aims at demonstrating the usage of software packages, and facilitating the exchange of information and ideas about known issues, possible developments, and future challenges in optical simulations.

The workshop concept stems from the international collaboration of optical simulation software developers from ESRF, ANL, BNL and Elettra. This began during the SPIE 2014 conference, and was further consolidated with a meeting at BNL in October 2015. The main goals of the collaboration are to share information about recent accomplishments and coordinate next efforts between leading teams in Europe and in USA in the area of software development for simulating SR/FEL Sources and X-Ray Optics.

The SOS workshop is not only suited for software developers or expert users, but also for scientists, researchers and students approaching the matter for the very first time. Thus it represents an opportunity to approach the optical simulation tools in a very effective way. The workshop could also be thought as an embryo of a possible future international school of Optics for Synchrotron Radiation.

A special session will be dedicated to industrial applications of optical simulations, in order to show usages, challenges and targets in different applied research fields.

SPONSORS

radiasoft

STRUMENTI SCIENTIFICI
CINEL® s.r.l.

DECTRIS®

KYMA

Rigaku

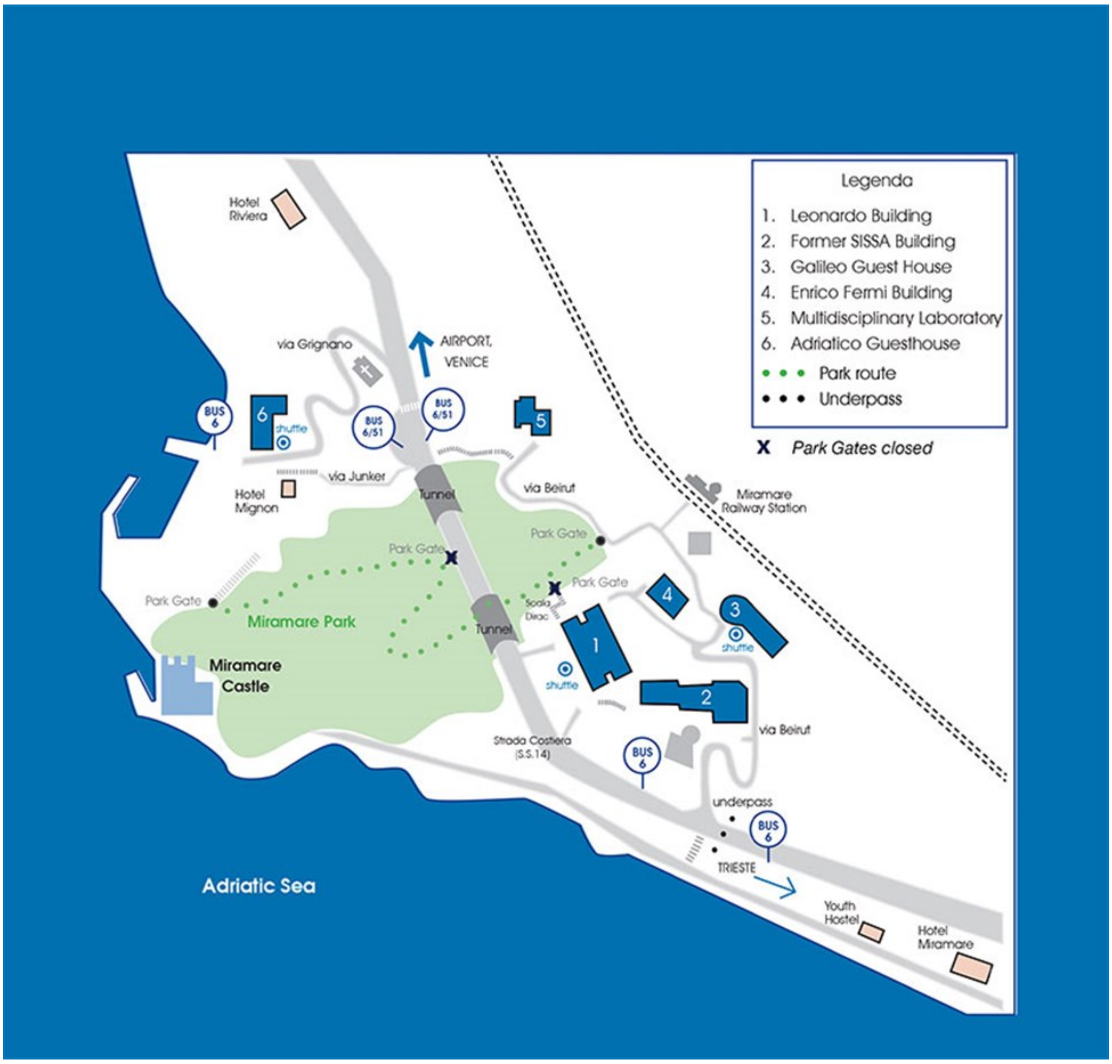
imagine optic™

WYROWSKI
PHOTONICS

AXO
AXO DRESDEN GmbH
APPLIED X-RAY OPTICS
MULTILAYER X-RAY OPTICS
HIGH PRECISION DEPOSITION

ICTP CAMPUS MAP

The ICTP campus is divided by the Strada Costiera, a busy thoroughfare connecting Trieste to Motorway A4. Narrow sidewalks and heavy traffic make walking along this road dangerous. There is a pedestrian crossing near the bus stops. Visitors are advised to strictly avoid crossing the road at other points, least of all in the tunnels.



ICTP Addresses

The Abdus Salam International Centre for Theoretical Physics (ICTP):

Address: Strada Costiera, 11 - 34151 Trieste, Italy
E-mail: pio@ictp.it
Tel: (+39) 040 2240 111 or 040 2240 + extension
Main fax: (+39) 040 224 163

SOS WORKSHOP PROGRAM

Monday, 3 October 2016

Welcoming
Room: ICTP - Leonardo Building Hall

09:00 ⇣	Registration

12:30 ⇣	*Lunch*

Ray-Tracing and Optical Calculation Tools
Chair: Luca Rebuffi
Room: Budinich Lecture Hall

13:45 ⇣	Luca Rebuffi *Introduction*
14:00 ⇣	Prof. Alfonso Franciosi - Elettra President and CEO *Welcome speech*
14:15 ⇣	Rami Sankari (MAX IV) *Simulations and design for soft-X-ray beamlines at MAX IV*
15:15 ⇣	Ruben Reininger (ANL) *Advances in Soft X-Ray beamlines design*

16:15 ⇣	*Coffee Break*

16:30 ⇣	Manuel Sanchez del Rio (ESRF) *Simulating hard x-ray beamlines by ray-tracing using ShadowOui*
17:30 ⇣ 18:00	Sergey Stepanov (ANL) *X-ray Server: dynamical X-ray diffraction on the web. Scope, history, capabilities, and future plans*

OASYS Helpdesk
Chair: Luca Rebuffi & Manuel Sanchez del Rio
Room: Adriatico Guest House – Meeting Room

20:00 ⇣ 22:00	Luca Rebuffi & Manuel Sanchez del Rio *Installation of OASYS on Mac, Linux and Windows*

Tuesday, 4 October 2016

Wavefront Propagation

Chair: Ruben Reininger
Room: Budinich Lecture Hall

09:00	Oleg Chubar (BNL) *High-Accuracy Partially- and Fully-Coherent Wavefront Propagation Calculations for Storage Ring and Free-Electron Laser Sources*
10:00	Xianbo Shi (ANL) *Partial Coherence, the Hybrid Method*
10:30	*Coffee Break*
11:00	Daniele Cocco (SLAC) *What you always wanted to have from a simulation software (and you never dare to ask for)*
12:00	Carsten Fortmann-Grote *Simulations of Experiments (SIMEX) work package in the European project EUCALL*
12:30	*Lunch*

Industrial Applications

Chair: Marco Zangrando
Room: Budinich Lecture Hall

14:00	Sara Paroni (Automotive Lighting Rear Lamps Italia S.p.A.) *Automotive lighting optical design and simulation: sequential and non-sequential ray-tracing*
14:40	Frank Wyrowski (Wyrowski Photonics) *Fast physical optics modeling of x-ray systems*
15:00	Sven Niese (Axo-Dresden) *Raytracing of real optics: tweaking the design of customized X-ray multilayer mirrors*
15:20	David Bruhweiler (Radiasoft) *An open source GUI for collaborative cloud-based X-ray optics modeling*
15:40	*Coffee Break*

16:00 ⇣	Guillaume Dovillaire (Imagine Optics) *Hartmann Wavefront measurement method and beamline alignment*
16:20 ⇣	Stefan Brandstetter (Dectris) *Hybrid Photon Counting Detectors for Current and Future Storage Rings*
16:40 ⇣	Riccardo Signorato (Cinel) *Strumenti scientifici CINEL: a reliable supplier for integrated optical components as well as a skillful partner for R&D projects*
17:00 ⇣ 17:20	Mirko Kokole (Kyma) *Optical calculations for the design of undulators at Kyma*

OASYS Helpdesk
Chair: Luca Rebuffi & Manuel Sanchez del Rio
Room: to de defined

20:00 ⇣ 22:00	Luca Rebuffi & Manuel Sanchez del Rio Installation of OASYS on Mac, Linux and Windows

Wednesday, 5 October 2016

Ray-Tracing: Soft X-ray SR-Beamlines
Chair: Sergey Stepanov
Room: Budinich Lecture Hall

09:00 ⇣	Ruben Reininger (ANL), Manuel Sanchez del Rio (ESRF) *Ray Tracing and Wave Propagation on Soft X-Ray beamlines design (part 1)*
10:30 ⇣	*Coffee Break*
11:00 ⇣ 12:30	Ruben Reininger (ANL), Manuel Sanchez del Rio (ESRF) *Ray Tracing and Wave Propagation on Soft X-Ray beamlines design (part 2)*
12:00 ⇣	*Lunch*

Ray-Tracing: Hard X-ray SR-Beamlines
Chair: Oleg Tchubar
Room: Budinich Lecture Hall

14:00 ⇣	Manuel Sanchez del Rio (ESRF), Luca Rebuffi (Elettra-Sincrotrone Trieste) *Simulating hard x-ray beamlines by ray-tracing using ShadowOui: Practical Session (part 1)*
15:30 ⇣	*Coffee Break*
16:00 ⇣ 17:30	Manuel Sanchez del Rio (ESRF), Luca Rebuffi (Elettra-Sincrotrone Trieste) *Simulating hard x-ray beamlines by ray-tracing using ShadowOui: Practical Session (part 2)*

Thursday, 6 October 2016

Wavefront Propagation: SR-Beamlines
Chair: Manuel Sanchez del Rio
Room: Budinich Lecture Hall

09:00 ⇣	Oleg Chubar (BNL) *Running Simulations with Synchrotron Radiation Workshop: from Web, under Python, in IGOR (part 1)*
11:00 ⇣	*Coffee Break*
11:30 ⇣	Oleg Chubar (BNL) *Running Simulations with Synchrotron Radiation Workshop: from Web, under Python, in IGOR (part 2)*
12:00 ⇣	Xianbo Shi (ANL), Luca Rebuffi (Elettra-Sincrotrone Trieste) *Practical session on Hybrid method within ShadowOui*
12:30 ⇣	*Lunch*

Wavefront Propagation: FEL
Chair: Marco Zangrando
Room: Budinich Lecture Hall

14:00 ⇣	Daniele Cocco (SLAC), Lorenzo Raimondi (Elettra-Sincrotrone Trieste), Cristian Svetina (Elettra Sincrotrone Trieste) *Practical session on FEL calculations with ShadowOui and WISE*
15:30 ⇣	*Coffee Break*
16:00 ⇣ 17:30	Liubov Samoylova *Practical session on XFEL calculations*
19:00 ⇣ 24:00	***Social Dinner***

Friday, 7 October 2016

Optical Calculation Tools
Chair: Daniele Cocco (SLAC)
Room: Budinich Lecture Hall

09:00 ⇣	Manuel Sanchez del Rio (ESRF) *Practical session on XOPPY*
10:30 ⇣	*Coffee Break*
11:00 ⇣	Sergey Stepanov (ANL) *A practical guide to accessing X-ray Server: web browser, scripting and XOPPY interfaces, adding new crystals and getting help*
12:30 ⇣ 12:45	Luca Rebuffi (Elettra-Sincrotrone Trieste) *Conclusion*

POSTER PERMANENT SESSION:
LIST OF ABSTRACTS
(ALPHABETIC ORDER BY AUTHOR)

RAY-UI: A Powerful and Extensible User Interface for RAY

P. Baumgärtel[1], M. Witt[2], J. Baensch[3], M. Fabarius[3], A. Erko[1],
F. Schäfers[1] and H. Schirmacher[3]
[1]Institute for Nanometre Optics and Technology
Helmholtz Zentrum Berlin für Materialien und Energie
Albert-Einstein-Str. 15, D-12489 Berlin, Germany
[2]Department Operation Accelerator BESSY II
Helmholtz Zentrum Berlin für Materialien und Energie
Albert-Einstein-Str. 15, D-12489 Berlin, Germany
[3]Fachbereich VI – Informatik und Medien
Beuth Hochschule für Technik Berlin,
Luxemburger Str. 10, D-13353 Berlin

email: peter.baumgaertel@helmholtz-berlin.de

The RAY-UI project started as a proof-of-concept for an interactive and graphical user interface (UI) for the well-known ray tracing software RAY [1]. In the meantime, it has developed into a powerful enhanced version of RAY that will serve as the platform for future development and improvement of the source code and associated tools [2].

The software as of today supports nearly all sophisticated simulation features of RAY. Furthermore, it delivers very significant usability and work efficiency improvements. Beamline elements can be quickly added or removed in the interactive sequence view. Parameters of any selected element can be accessed directly and in arbitrary order. With a single click, parameter changes can be tested and new simulation results can be obtained. All analysis results can be explored interactively right after the ray tracing by means of powerful integrated image viewing and graphing tools. Unlimited image planes can be positioned anywhere in the beamline, and bundles of images planes can be created for moving the plane along the beam to identify the focus position with live updates of the simulated results.

In addition to showing the features and workflow of RAY-UI, we will give an overview of the underlying software architecture as well as an outlook for future developments.

Installers of RAY-UI are available for Windows, Mac OSX and Linux on our homepage: http://hz-b.de/ray

References:

[1] F. Schäfers, RAY - The BESSY Raytrace Program, in: Modern Developments in X-Ray and Neutron Optics, Springer Series in Modern Optical Sciences, eds A. Erko, , M. Idir, Th. Krist, , A.G. Michette, Vol. **137**, 9-41 (2008)

[2] P. Baumgärtel, M. Witt, J. Baensch, M. Fabarius, A. Erko, F. Schäfers and H. Schirmacher, RAY-UI: A Powerful and Extensible User Interface for RAY, AIP Conf. Proc. **1741**, 040016 (2016)

The LAUPER project (LAUe-PEak Radiotherapy)

Bellucci Valerio[a], Mazzolari Andrea[a], Cardarelli Paolo[a], Di Domenico Giovanni[a],
Gambaccini Mauro[a], Guidi Vincenzo[a], Camattari Riccardo[a], Marziani Michele[a],
Paternò Gianfranco[a], Taibi Angelo[a], Baldazzi Giuseppe[b], Lanconelli Nico[b],
Morigi Maria Pia[b], Peccenini Eva[b], Spighi Roberto[b]

[a] Department of Physics and Earth Sciences, University of Ferrara, Via Saragat 1/c, 44122 Ferrara, and INFN section of Ferrara, Italy.

[b] Department of Physics and Astronomy, University of Bologna, Viale Berti Pichat 6/2, 40127 Bologna, and INFN section of Bologna, Italy

email: valerio.bellucci@unife.it

The LAUPER project aims to demonstrate the feasibility of a Laue lens optimized to operate with X-rays emitted by a conventional X-ray tube to produce a focused photon beam for radiotherapy applications. In the context of tumor treatment, radiotherapy is an important method consisting in imparting a radiation dose to a target volume in order to destroy cancer cells. Any radiotherapy treatment aims to maximize the dose to the target volume, minimizing at the same time the irradiation of neighboring healthy tissues. Among radiotherapy treatments, hadron therapy uses charged particles beams, namely protons or positive ions, to achieve the aforementioned goal. Indeed, positive ions have a finite range of penetration in a tissue and a high amount of energy released at the end of their track (the Bragg peak). However, the cost of a facility for hadron therapy is very high, at least 100 M€. Only a few dozen of hadron therapy facilities exist in the world, and half of them are concentrated in the United States and in Japan. Thus, only a limited number of patients can access to the high-quality treatment provided by hadron therapy. Conventional radiotherapy relies on electron linear accelerator producing photon beams in the MeV energy range to reach the tumor target and spare the skin. However, such technique is not comparable with the hadron therapy in terms of dose deposition accuracy. The cost of a facility for conventional X-ray treatments ranges in 1-2 M€. A device capable of focusing X-rays would allow concentrating the delivered dose in a target volume. Due to focalization, the photon flux would increase with the penetration depth in the tissue and would reach the maximum at the focal point. The combination of this effect with the photon absorption would give rise to a depth-dose profile showing a pronounced peak at focal point and a rather rapid fall-off beyond this point. This behavior resembles that of a Bragg peak, typical of hadron therapy, resulting in a “Laue peak”. In order to concentrate an X-ray beam, the phenomenon of diffraction can be exploited. A proposed optics is the Laue lens, namely an ensemble of crystals arranged in concentric rings and disposed in such a way to diffract as much radiation as possible toward the focal point of the lens, where the tumor mass is positioned. Such a focusing device can be used together with a conventional X-ray tube to focus photons in the energy range 25-250 keV. Thus, it would be possible to reach high precision in the dose delivery with an equipment orders of magnitude less expensive if compared to the cost of a facility for hadron therapy. Indeed, the cost of such equipment would be in the range of 0.2-0.3 M€, even less expensive than the equipment for traditional radiotherapy based on MeV X-ray beams. During this project, we aim to construct a crystal assembly capable of diffracting an 80 keV X-ray beam and producing the aforementioned Laue peak in a proper phantom.

The software spectrum for optical simulation @ SOLEIL

David Dennetiere[1], Thierry Moreno[1], François Polack[1]
[1] *Synchrotron Soleil, L'Orme des Merisiers, Saint-Aubin, 91192 Gif-sur-Yvette, France*

email: david.dennetiere@synchrotron-soleil.fr

Over the years, the SOLEIL optics group needs have evolved from designing beamline with micrometer spot size to designing beamline with nanometre spot size. The instruments around the experiments have also deeply evolved. As the tasks got more and more diverse, many optical simulation tools have been used, developed and upgraded.

The result is a broad spectrum of software ranging from one shot program to commercial programs including several in house developed reflectivity and ray-racing software. As versatile and handy this tool suite presently is, the question of maintaining all these codes is raised. Some of the developers have left, and some codes have become barely upgradable because of their bulkiness, their reliance on obsolete libraries, and the convoluted structure as over time coders have stacked layers upon layers. Their probable obsolescence is becoming more and more a challenge that needs to be addressed.

The different software and their uses will be presented as well as our vision for the future of code development at SOLEIL in a long-time support perspective.

Optical Design of Powder Diffraction Beamline for ILSF

A. Gholampour Azhir
Institute for Research in Fundamental Sciences, Iranian Light Source Facility

Azam.gholampour@ipm.ir

Iranian Light Source Facility (ILSF) project has been initiated since 2010 in order to design and construction of a third generation synchrotron facility with 3 GeV energy, 400 mA electron current, 0.28 nm.rad horizontal emittance for developing basic and engineering researches in Iran [1]. In parallel to the design and construction of the accelerator machine, a scientific division has been formed to reach the purpose of capacity building, organizing the users' community, design and construction of the ILSF beamlines. Seven day-one beamlines with its users' requirements has been specified by the users' community. X-ray Powder Diffraction beamline is one of the first priorities of the Iranian Light Source Facility day-one beamlines. This beamline will cover the research requirements of scientific community in the fields of physics, material science, chemistry, etc. Scope of design of this beamline is to meet the Iranian users' requirements such as energy range: 6-30 keV, flux: 10^{12} ph/s, energy resolution: 10^{-4} and spot size at sample: 0.1×0.1-10×1 mm^2. In this report type of the source, optical elements and their specifications have been discussed. Ray tracing calculations from source to sample, and optimization of the parameters have been done [2-6].

References

[1] ILSF CDR: http://ilsf.ipm.ac.ir/Publications/ILSF-CDR.pdf
[2] H. Wiedemann. "Synchrotron Radiation", Springer, 2002.
[3] B.D. Patterson et al, " the materials science beamline at the Swiss light source", Nuclear Instruments and Methods in Physics Research A 540, 42–67, (2005)
[4] M. Knapp, I. Peral, " Conceptual design report of the materials science and powder diffraction beamline MSPS at ALBA", 2007.
[5] T.Tanaka and H. Kitamura, J. Synchrotron radiation, No. 8 ,1221 (2001).
[6] www.esrf.eu/usersand science/experiments/TBSscisoft/xop2.3

Simulation and Reconstruction of Coherent Modes for Near Field Imaging

Johannes Hagemann and Tim Salditt
Institute for X-ray physics, Friedrich-Hund-Platz 1, University Göttingen,
37077 Göttingen, GERMANY

email: jhagema@gwdg.de, tsaldit@gwdg.de

In X-ray near field imaging experiments the probing beam determines the imaging quality in terms of resolution and artifacts. Distortions in the probe from optical elements such as focusing optics can easily spoil quantitative contrast. Thus characterizing the probe is an important issue. In previous work [1] we have reconstructed the probe under the assumption of full coherence. In this contribution we extend the reconstruction scheme to include also the partial coherent case, by extending the ptychography approach proposed for far field detection [2] to the near field. The reconstruction scheme uses the measurements from multiple detection planes. Experimentally this is achieved by moving the detector to different distances. The reconstruction is numerically quite demanding since the modes have to be individually propagated and orthogonalized in each iteration of the reconstruction algorithm. Without the use of GPUs this would be a time consuming process. By numerical simulations and a suitable representation of modes, we show how to take into account partial spatial coherence, both in image formation and in reconstruction. Our results show that the occupation numbers of the modes and the degree of coherence can be reconstructed.

References:

[1] J. Hagemann et al., J. Synchrotron Radiat., submitted.

[2] P. Thibault, A. Menzel, Nature **494,** 68-71(2013).

The optical scheme of the ESRF soft X-ray beamline ID32

K. Kummer[1], F. Yakhou-Harris[1], N.B. Brookes[1]
[1]*ESRF-The European Synchrotron, 71 Avenue des Martyrs, Grenoble, France*

email: kurt.kummer@esrf.fr

We will present the optical scheme of the ID32, the ESRF soft X-ray beamline including ray tracing and commissioning results. The beamline is working in the soft X-ray range between 400 eV and 1600 eV. It had to accommodate two branches with very different requirements but sharing the same plane VLS grating monochromator. The branch for XMCD-type experiments required a moderate resolving power between 5,000 and 10,000 but optimization for easy operation and on-the-fly energy scans across the entire working range of the beamline. The second branch is dedicated to high-resolution resonant inelastic X- ray scattering (RIXS) and needed to be optimized for extremely high-resolving powers and flux. This led for the XMCD branch to an optical design that has not been considered for a soft X-ray absorption beamline before. Both branches of the beamline are now in user operation and performing as expected.

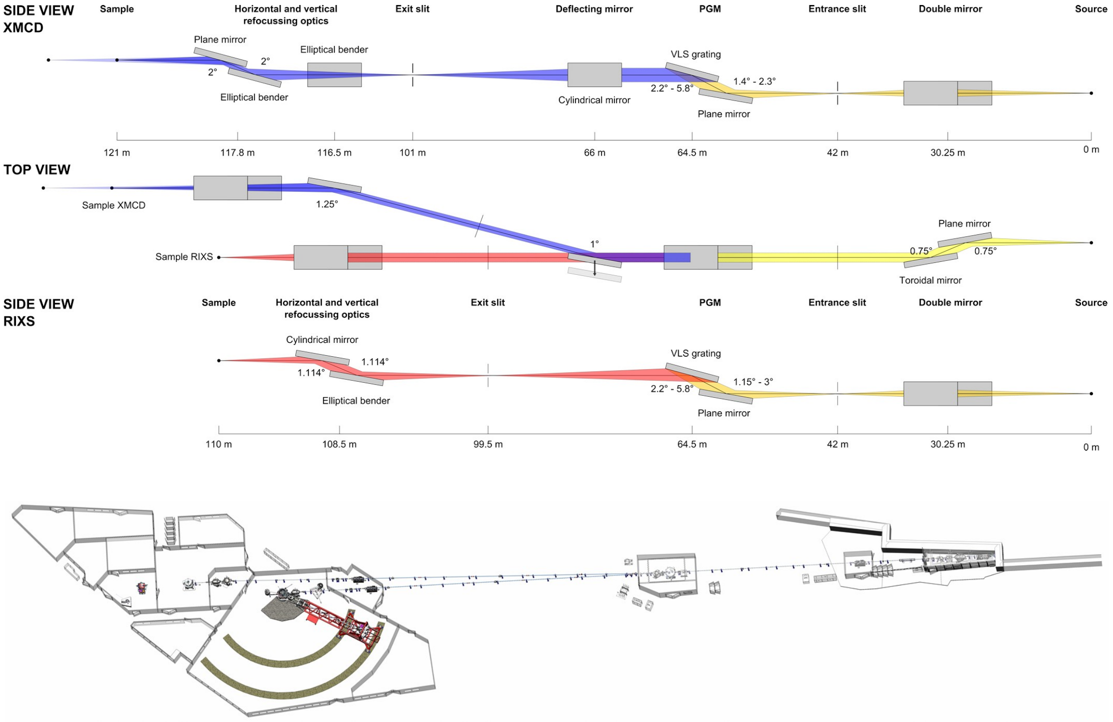


Figure caption: Optical and floor layout of the ESRF soft X-ray beamline ID32 with two branches dedicated to high-resolution RIXS and to XMCD-type experiments.

Selecting the coherent fraction of low emittance synchrotrons

Sérgio Lordano[1], Bernd Meyer[1], Florian Meneau[1], Harry Westfahl Jr.[1]
[1]*Brazilian Synchrotron Light Laboratory, 10.000 Giuseppe Máximo Scolfaro, Campinas, 13.083-970, BRAZIL*

email: sergio.lordano@lnls.br

In this work we study the coherence properties of a synchrotron beam emitted by an undulator, which is the greatest feature of ultra-low emittance 4th generation storage rings. In the frame of wave optics, we use Synchrotron Radiation Workshop (SRW) [1] to simulate the mutual coherence function of a smoothly focused beam, which is measured directly by the propagation of the beam through a Non-Redundant Array (NRA) of slits [2]. With this approach it is possible to time-efficiently retrieve the coherence length at the focal position in a single-shot simulation, instead of a set of double-slit experiments. The results are compared to the Gaussian-Schell model analytical predictions [3], which agrees well quantitatively, if the equivalent Gaussian beam dimensions are properly calculated by the universal function. It is also shown the effects of increasing the beam degree of coherence by limiting the beam divergence with hard-edge slits, which can turn even achromatic focusing systems into chromatic, accounted for in both analytical and numerical methods. The effect of optics figure errors on the coherence properties of the beam can be exploited in this method, and allows realistic and efficient optical design of beamlines and components of the next generation light sources. Work submitted to J. Synchrotron Rad. [4].

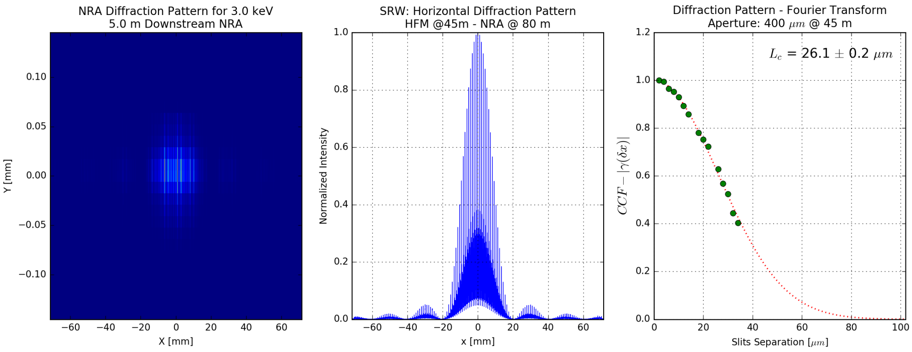


Figure 1: 2D Diffracted beam (left), horizontal cut (center) and measured correlation function (right), 5 m downstream the NRA.

References:

[1] O. Chubar, P. Elleaume, Proceedings of EPAC-98, 1177-1179 (1998).

[2] I. A. Vartanyants et al, J. Synchrotron Rad. **21**, 722-728 (2014).

[3] A. Singer, I. A. Vartanyants, J. Synchrotron Rad. **21**, 5-15 (2014).

[4] H. Westfahl Jr. et al, submitted to J. Synchrotron Rad.

Paraxial propagation of x-rays in matter beyond the stationary approximation

Lars Melchior[1], Tim Salditt[1]
[1]*Universität Göttingen - Institut für Röntgenphysik, Göttingen, 37077, GERMANY*

email: lars.melchior@stud.uni-goettingen.de

Full wave-optical simulations of wavefield propagation are needed for a multitude of x-ray optical problems - from the design of instruments (refractive lenses, diffractive optics, waveguides) and experiments to data analysis and reconstruction of thick samples and objects. At the same time, numerical propagation is extremely challenging in free space and even more so in matter. Finite difference equations of the paraxial wave equation have been demonstrated as an efficient tool for stationary wavefield propagation, as described in Fuhse [1]. In this work, we extend numerical simulations of paraxial wave propagation beyond the stationary case, including for example dispersion properties of ultra-fast x-ray pulses relevant for FEL experiments. We first address suitable formulations and approximations on the level of the equations, then present an efficient numerical framework for the general case of both stationary and non-stationary problems, and finally benchmark the numerical results with exact analytical solutions.

To perform these tasks, we introduce the PyPropagate framework, as a high-performance paraxial wave propagation package for python, which can be used for any user-defined distribution of matter (in the continuous model) and arbitrary boundary conditions, both in 2D and 3D configurations. By combing a multi-core C++ backend with a sophisticated computer algebra system and just-in-time compilation we can achieve very high performance on almost every system. Additionally, this allows us to keep the required user input to a minimum while making the simulation framework accessible to users with none or little programming experience. Typical working times on a 2011 consumer notebook are seconds for 2D - and minutes for 3D - stationary solutions.

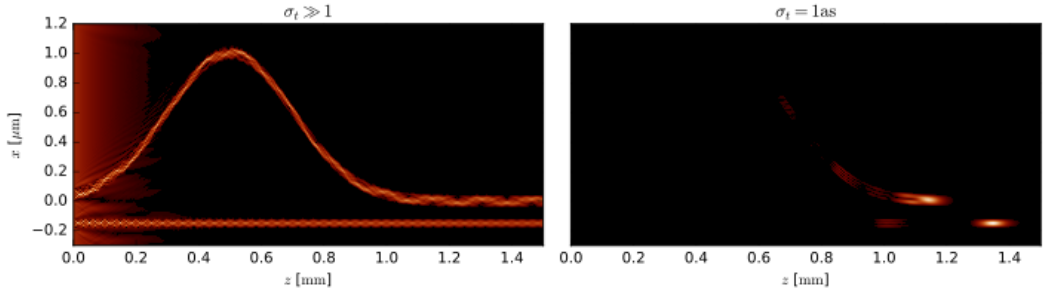


Figure caption: Illustration of (left) stationary and (right) time-dependent wavefield intensity in straight and curved waveguide channels in Germanium at 12keV to determine the time delay.

References:

[1] Fuhse, Christian. X-ray waveguides and waveguide-based lensless imaging. Universität Göttingen - Institut für Röntgenphysik. 2006.

Characterizing the Nanofocus beamline Carnaúba of SIRIUS by ray-tracing (SHADOW) and wave-propagation (SHADOW-HYBRID, SRW) simulation

Bernd Meyer[1], Sergio Lordano[1], Helio Tolentino[1], Harry Westfahl Jr.[1]
*[1]Brazilian Synchrotron Light Laboratory, 10.000 Giuseppe Máximo Scolfaro, Campinas,
13.083-970, BRAZIL*

email: bernd.meyer@lnls.br

The Carnaúba (Coherent X-Ray Nanofocus Beamline) beamline [1] at SIRIUS synchrotron is dedicated to x-ray scattering, absorption and fluorescence techniques using coherent photons focused at a nanometric scale. The optics provide a focal spot at the experimental station of ~30 nm with a working distance of ~6cm. This work presents the optical concept of the Carnaúba beamline. We discuss the results of the geometrical ray-tracing (SHADOW3 [2]) and of the wave-propagation (SHADOW-HYBRID and SRW [3],[5]). It is shown that the surface error profile overestimates the beam size using the ray-tracing method. For sub-micrometre focal spot size wave-propagation is mandatory. Aperture sizes and the size of the optical elements must be defined carefully, as focal distances change due to diffraction effects at those apertures. SHADOW's Hybrid method is used efficiently to specify all parameters. As wave-propagation simulations by SRW are very time-consuming, we compare and verify the simulations for selected cases with SHADOW's Hybrid method.

References:

[1] Tolentino, Helio. "Carnaúba Beamline: Preliminary Design Report (PDR)". Unpublished
[2] M. Sanchez del Rio, N. Canestrari et al, J. Synchrotron Rad. **18**, 708-716 (2011).
[3] X. Shi, R. Reininger et al, SPIE **9209**, 920909 (2014).
[4] X. Shi, R. Reininger et al, J. Synchrotron Rad. **21**, 669-678 (2014).
[5] O. Chubar, L. Berman et al, SPIE **8141**, 814107 (2011).

Combining electron beam dynamics and x-ray optics codes for Synchrotron light sources

Boaz Nash[1], Manuel Sanchez del Rio[1], Mark Glass[1]
[1]*ESRF Grenoble, FRANCE*

email: boaz.nash@esrf.fr

Calculations of x-ray propagation down synchrotron beamlines require knowledge of the electron beam at the source point and details of the undulator or bending magnet magnetic field. The electron source properties are typically calculated independently, using electron beam dynamics codes which are used for the lattice design for new synchrotrons, or tuning of existing synchrotrons. The resulting electron beam parameters are used as inputs to the x-ray simulations. Here we propose a tighter integration between electron beam source calculations and synchrotron radiation calculations down beamlines.
We describe the second moment electron beam calculation using the Ohmi Envelope method1 as implemented in the Accelerator Toolbox (AT) Matlab based beam dynamics code2. We mention several cases where the usual input to x-ray codes of Twiss parameters and emittances may be inadequate, namely, x-y coupling, energy spread effects, and non-Gaussian electron beams, such as with harmonic RF cavities for bunch lengthening.

For beam dynamics calculations, we focus on the AT code. This code is open source, and is developed by accelerator scientists at numerous labs. A SourceForge repository (atcollab) exists, as does a mailing list for communication. A python version has just started development. We suggest how this code may be integrated with existing efforts at a larger framework for x-ray optics computation such as the OASYS project3.

References:

[1] Ohmi et. al. “From the beam-envelope matrix to synchrotron-radiation integrals” Phys. Rev. E 49, 751 (1994)

[2] B. Nash et. al, “New Functionality for Beam Dynamics in Accelerator Toolbox (AT)”, Proc. IPAC ‘15

[3] M. Sanchez del Rio, L. Rebuffi, J. Demšar, N.Canestrari and O. Chubar, "A proposal for an open source graphical environment for simulating X-ray optics", Proc. SPIE 9209, 92090X (2014)

Aberrations in compound refractive lens systems: analytical and numerical calculations

Markus Osterhoff[1], Carsten Detlefs[2], Claudio Ferrero[2]
[1]*Institute for X-Ray Physics, University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany*
[2]*European Synchrotron Radiation Facility, 71 Avenue des Martyrs, 38000 Grenoble, France*

email: mosterh1@gwdg.de

One famous optical system at synchrotron sources are compound refractive lenses (CRLs) that allow for focus sizes on several micrometre down to sub-100 nm. In case of transfocators, the actual number of lenses can be changed to match the required focal length and beam size for various x-ray energies [1]. Typical setups use tens to up to one hundred of individual lenses. But beam quality of such CRL stacks can suffer from fabrication errors of the individual lenses, from stacking errors in one CRL cartridge of two up to 128 lenses, and from a misalignment of cartridges with respect to each other. One common problem of single lenses are deviations from the ideal shape (in thin lens approximation, rotational paraboloids); but a single lens can also be misplaced laterally to the optical axis, or tilted with respect to the incoming beam. Lenses inside stacks and the cartridges of transfocators can also be both misplaced and tilted; as these alignment errors can correlated, their impact on beam quality can be enhanced by two orders of magnitude compare to random errors of singles lenses.

These shape and alignment errors cause aberrations or wave-front errors. We have expanded typical single-lens errors in a series of Zernike polynomials [2]. After an analytical description for single lenses is given and interpreted, acceptable alignment tolerances and error bounds for both independent and correlated stacking errors are given based on numerical simulations. The numerical investigations use a new C library for Zernike polynomials that allows to both superpose model aberrations and to project numerically given phase fronts onto a basis of Zernike phase polynomials to calculate the series expansion coefficients.

References:

[1] G.B.M. Vaughan, J.P. Wright, A. Bytchkov, M. Rossat, H. Gleyzolla, I. Snigireva, A. Snigirev, J Synchrotron Radiat **18**, 125-133 (2011).

[2] Max Born, Emil Wolf. Principles of Optics. Cambridge University Press (7th edition), 1999.

Simulations and design for soft X-ray beamlines at MAX IV

Rami Sankari[1]
[1]*MAX IV Laboratory, Lund University, P.O. Box 118, 221 00 Lund, SWEDEN.*

email: rami.sankari@maxiv.lu.se

MAX IV Laboratory, under construction in Lund Sweden, has two storage rings operated at 3 GeV and 1.5 GeV and optimized for the hard and soft x-ray/VUV energy ranges, respectively [1]. The multibend achromat lattice employed for the 3 GeV allows to achieve very low emittance, c.a. 0.2 nm·rad in relatively small ring, circumference being 528 m with a straight section length of 4 m. For the 1.5 GeV ring, the magnet design is similar, based on compact integrated magnet structure, but forming a double bent achromat lattice instead. The emittance for this 96 m circumference ring is c.a. 6 nm·rad and it has twelve 3 m long straight sections.

The low emittance combined with relatively high electron beam current results in high-power, low-divergence beams. With reasonable opening angle towards the beamline, the power is typically in the kW regime, and for grazing incidence optics the maximum power density approaches 1 W/mm^2. The optical elements exposed to high heat load are cooled internally by water flow and whereas the modeling for thermal stability is feasible, the mechanical effects of turbulent flow in a mirror and its support is a more difficult question.

Another consequence of low emittance is that Gaussian approximation often used for undulators is not valid anymore. This is well described theoretically (see e.g. Ref. [2]) but precise modeling within the ray tracing programs are still rare, although the actual shape and divergence of the source play an important role when pushing the performance of the beamlines further.

Finally, transverse coherence is also connected to the low emittance, and one of the beamlines presented here is aimed for coherent imaging; modeling the degree of coherence, and coherence lengths at the sample plane became a question, which in this case is solved by utilizing a modeling tool developed partly at MAX IV, the XRT-package [3].

References:

[1] P. Tavares, S. Leemann, M. Sjöstrom, and Å. Andersson, J. Synchrotron Rad. 21, 862 (2014).

[2] P. Elleaume in: *Undulators, wigglers and their applications*, Eds. H.Onuki and P. Elleaume,
Taylor & Francis, 69-108 (2003).

[3] K. Klementiev and R. Chernikov, Proc. SPIE 9209, 92090A (2014).

MASH, a Framework for the Automation of X-ray Optical Simulations

Peter Sondhauss[1]
[1]*MAX IV Laboratory, Lund University, P.O. Box 118, 221 00 Lund, SWEDEN.*

email: peter.sondhauss@maxiv.lu.se

MASH stands for "Macros for the Automation of SHadow". It allows to run a set of Shadow3 ray-tracing simulations, e.g. for a range of photon energies, fully automatically. Undulator gaps, crystal angles etc. are tuned automatically. Important output parameters, such as photon flux, photon irradiance, focal spot size, bandwidth, etc. are then directly provided as function of photon energy. A photon energy scan is probably the most commonly requested, but any parameter or set of parameters can be scanned through as well.

Heat load calculations with finite element analysis providing temperatures, stress and deformations (Comsol) are fully integrated. The deformations can be fed back into the ray-tracing process simply by activating a switch.

MASH tries to hide program internals such as file names, calls to pre-processors etc. so that the user (nearly) only needs to provide the optical setup. All input parameters are stored in a single human-readable file in XML format.

MASH comes with a web interface, which allows to run it remotely on a central computation server. Hence, no local installation or licenses are required, just a web browser and access to the local network. On the computation server, the only commercial license required is that for the finite element code Comsol.

Numerous tools are provided to examine the ray-tracing results in the web-browser. The results can be also downloaded for local analysis. All files are human readable text files that can be easily imported into third-party programs for further processing.

A useful feature, in particular for those who run many simulations for others, is a heavily configurable automatic report generation, including tables with the most relevant setup parameters, a schematic of the optical setup, plots of result statistics (e.g. flux as function of photon energy), false colour images of photon irradiance, etc.

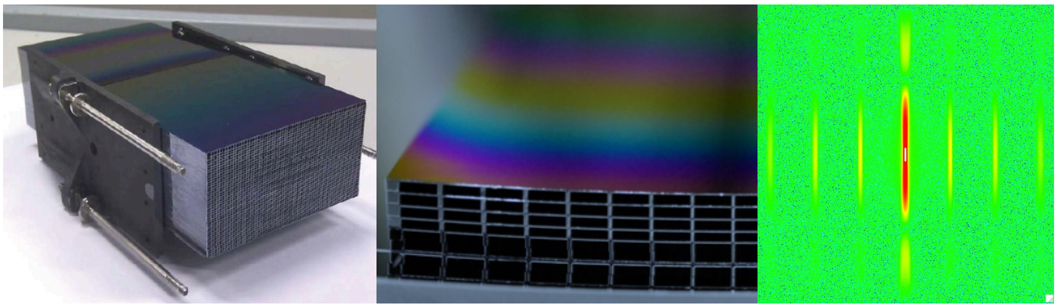
Diffraction simulations of silicon pore optics for the ATHENA X-ray telescope

D. Spiga[1], F.E. Christensen[2], M. Bavdaz[3], G. Bianucci[4], M.M. Civitani[1], P. Conconi[1],
D. Della Monica Ferreira[2], F. Marioni[4], S. Massahi[2], G. Pareschi[1], B. Salmaso[1],
B. Shortt[3], K. Tayabaly[1,5], G. Valsecchi[4], N.J. Westergaard[2], E. Wille[3]

[1] INAF – Brera Astronomical Observatory, Via Bianchi 46, Merate, 23807, ITALY
[2] DTU Space, Techn. Univ. of Denmark, Elektrovej, bygn. 327, Kgs. Lyngby, 2800, DENMARK
[3]European Space Agency, ESTEC, Keplerlaan 1, Noordwjik, 2201 AZ, THE NETHERLANDS
[4]Media Lario Technologies, loc. Pascolo, Bosisio Parini, 23842, ITALY
[5]Politecnico di Milano, Via La Masa 1, Milano, 20156, ITALY

email: daniele.spiga@brera.inaf.it

The ATHENA X-ray observatory is a large-class ESA selected mission, with launch scheduled in 2028. The technology of silicon pore optics (SPO) [1] was selected as baseline to assemble ATHENA's optic with more than 1000 mirror modules, obtained by stacking wedged and ribbed silicon wafer plates onto silicon mandrels to form the Wolter-I configuration [2]. The stringent requirement of a 5 arcsec HEW angular resolution at 1 keV entails very small profile errors and excellent surface smoothness, as well as a precise alignment of the 1000 mirror modules in a 3 m diam. optical assembly to avoid imaging degradation and effective area loss. Such an accurate alignment is difficult to perform in X-rays because a very broad, parallel beam, and a handling device under high vacuum would be necessary. The module handling and alignment is much easier to achieve in air using UV light, even if the densely stacked and ribbed structure of SPOs represents a major source of aperture diffraction. In order to understand if the center of mass of the UV diffraction pattern is a reliable marker of the expected focus location in X-rays, we deal with a detailed description of diffractive effects expected in an SPO module [3] on the basis of the Fresnel diffraction theory in far-field approximation. We also show an interesting comparison with real data measured in an UV optical bench.



Left: one of the silicon pore optics ofr the ATHENA X-ray telescope mirror assembly [1]. Center: a closer view on the aperture of a module showing the densely ribbed structure [2]. Right: a diffraction pattern simulation at 220 nm light wavelength [3].

References

[1] Bavdaz, M., Wille, E., Shortt, B., Fransen, S., et al., Proc. SPIE 9905, 990527 (2016)

[2] Collon, M., Vacanti, G., Guenther, R., et al., Proc. SPIE 9905, 990528 (2016)

[3] Spiga, D., Christensen, F.E., Bavdaz, M., et al., Proc. SPIE 9905, 99055O (2016)

Profile measurement delivery of European XFEL long flat mirrors using Fizeau interferometry

Maurizio Vannoni, Idoia Freijo Martín, Harald Sinn
European XFEL GmbH, Holzkoppel 4, 22869 Schenefeld, Germany

email: maurizio.vannoni@xfel.eu

The European XFEL will generate extremely short and intense X-ray laser pulses of high coherence with a nearly diffraction-limited beam. To guide these X-rays beams over a distance of more than 1 km to the experimental hall requires very flat mirrors to have a good control of the divergence of the beam. The specifications of the X-ray mirrors that will be used for this purpose, to transport, distribute and focus the beam, are therefore highly demanding. It will be required for the reflecting surfaces to have a surface quality better than 2 nm Peak-To-Valley over a 950-mm length. In order to account for the real shape of the mirrors in a fast and reliable way it is proposed to use a Fizeau interferometer. The mirrors are much bigger than the interferometer clear aperture, so it is needed to use an angled ("grazing incidence") cavity setup to be able to measure the mirrors over their entire length. Complementary, a stitching method is also used.

We present some preliminary results about the measurements carried out so far, using the present capabilities of the Metrology Lab at European XFEL. The mirrors examined are with final polishing but before the required coating. Together with the results, we summarize the future activities that will be required to perform the best characterization of the final systems before installation.

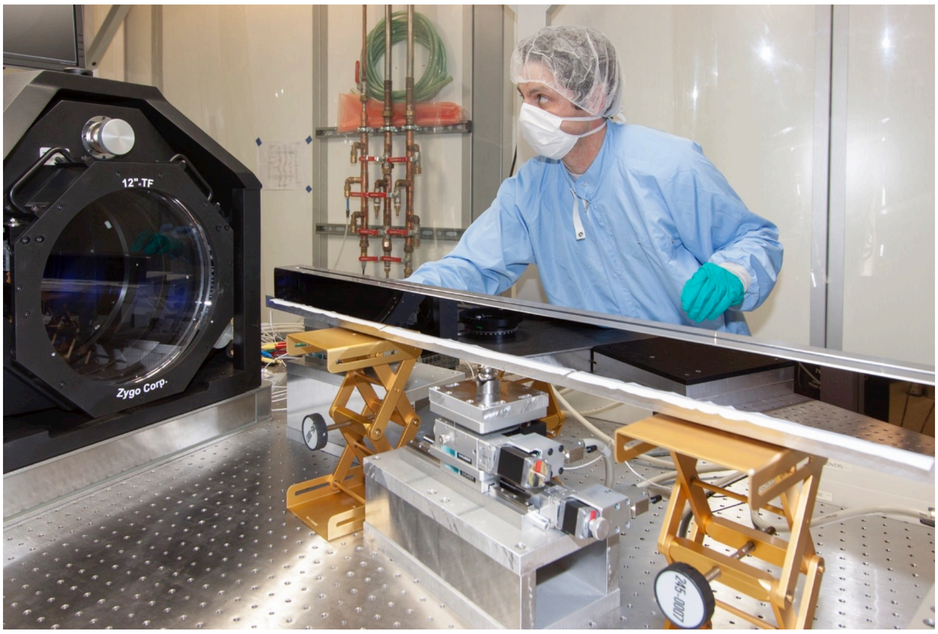


Figure caption: Inspection of one of the beam transport mirrors (http://goo.gl/79AK63)

References:

[1] M. Altarelli et al., Technical Design Report, DESY 2006-097, (July 2007).

[2] M. Vannoni and I. Freijo Martín, Rev. Sci. Instrum. **87**, 051901 (2016).

[3] M. Vannoni and I. Freijo Martín, Metrologia **53**(1), 1–6 (2016).

Fast physical optics modeling of x-ray systems

Frank Wyrowski[1,3], Antonie Verhoeven[2], Christian Hellmann[3]
[1]*University of Jena, Jena, 07743, GERMANY.*
[2]*University of Eastern Finland, Joensuu, 80101, FINLAND.*
[3]*Wyrowski Photonics UG, Jena, 07745, GERMANY.*

email: frank.wyrowski@uni-jena.de

Optical modeling and design on the basis of physical optics is of increasing concern for the modeling of x-ray beamlines. Physical optics deals with electromagnetic fields which are governed by Maxwell's equations. Solving Maxwell's equations is often understood to be not practical for real optical and x-ray systems. That is true if we try to tackle the problem with an universal Maxwell solver like for instance FDTD. Though such solvers are great mathematical and numerical tools, they allow the solution of Maxwell's equations just in subdomains smaller than about $(100\ \lambda)^3$. We have introduced the concept of field tracing to deal with this challenge in physical optics modeling [1]. In field tracing the system is decomposed into different subdomains in which different techniques to solve Maxwell's equations are applied. Starting from the source fields the fields are traced through the system by solving a sequence of boundary value problems. That can be extended to a non-sequential technique which provides a solution of Maxwell's equations in the entire system [2]. In short the concept can be understood as a significantly generalized S-matrix approach. It mainly benefits from the combination of geometric and diffractive techniques [3][4]. The geometric techniques are as fast as ray tracing and in subdomains in which diffractive techniques are demanded, e.g. in the focal zone of a field, the diffractive techniques can often benefit from FFT based methods. That results in a fast and practical physical optics modeling concept, which includes all electromagnetic field phenomena like polarization, interference, diffraction and partial coherence.

The modeling of practical sources requires the inclusion of partial coherence. We model partial coherence by a mode decomposition of the source field. Each mode can be propagated by field tracing. This approach has turned out to be very beneficial.

X-ray radiation represents an electromagnetic field and thus it can be propagated by field tracing through x-ray systems. We have started to investigate the special constraints and challenges which come with x-ray modeling and like to present our first results at the meeting. We plan to use your feedback and the discussions to add those features to our fast physical optics software Virtuallab Fusion which makes it to a powerful tool for the x-ray community [5].

References:

[1] F. Wyrowski, M. Kuhn, Introduction to field tracing, J. Mod. Optics **58**, 449-466 (2011)

[2] M. Kuhn, F. Wyrowski, C. Hellmann, Non-sequential optical field tracing, in Advanced Finite Element Methods and Applications, Springer Berlin Heidelberg, 257-273 (2013)

[3] F. Wyrowski, et al., Approximate solution of Maxwell's equations by geometrical optics, Proc. SPIE 9630, 963009 (2015)

[4] F. Wyrowski, C. Hellmann, Geometrical optics reloaded, Optik&Photonik **10**, 43-47 (2015)

[5] Physical optics software "Wyrowski VirtualLab Fusion", developed by Wyrowski Photonics UG, distributed and supported by LightTrans GmbH, Jena, Germany.

Using SimEx platform in HPC environments

Sergey Yakubov[1], Carsten Fortmann-Grote[2]
[1] DESY, Notkestrasse 85, Hamburg, 22607, GERMANY.
[2]European XFEL, Holzkoppel 4, Schenefeld, 22869, GERMANY.

email: sergey.yakubov@desy.de

Photon experiment simulation platform SimEx [1] is being developed in the framework of the European Cluster of Advanced Laser Light Sources (EUCALL) project. It implements a full start-to-end simulation of experiments at various light sources like free electron lasers. The simulations embrace all the steps of the experiment: from generation of radiation in the photon source, propagation trough the optic and waveguides to the interaction point, photon-matter interaction, scattering of the radiation in the far field and detection of the latter. Samples range from weakly scattering biomolecules, density modulations following laser–matter interaction to dynamically compressed matter at conditions similar to planetary cores.

SimEx provides basic computation modules (calculators) tailored for simulation of coherent diffractive single particle imaging and an interface to add/replace calculators in the experiment chain for other use cases. A common data format based on the HDF5 library is developed for data exchange between calculators.

SimEx simulations may take weeks or months to finish when run on a single machine. To be able to get results in a more reasonable wall-clock time SimEx platform has to be adapted for deployment and parallel simulations on an HPC cluster. This is not a trivial task due to diversity of codes used for various calculators. Thus, some calculators use legacy code developed for use on a single-core machine, whereas other calculators can efficiently run on GPU cards. Moreover, all calculators have their own third-party dependencies and install scripts, which make deployment process overcomplicated.

To facilitate SimEx deployment, several options are available. One can install SimEx from sources from GutHub [1] using CMake build system. CMake checks all dependencies before installation, informs a user if some libraries are missing, finds and installs all available calculators. Alternatively, binary packages are created for various platforms and are also available on GitHub. Finally, SimEx Docker image can be provided to automate the deployment inside software containers. For HPC clusters installation via CMake system seems most appropriate, unless HPC cluster can operate with Docker containers.

Parallelization of SimEx calculators is now in a progress. The SRW library used for the wavefront propagation calculator is efficiently parallelized with hybrid OpenMP/MPI approach and showed 160x simulation speed-up on our in-house HPC cluster. More results will be presented during the workshop.

References:

[1] SimEx platform repository on GitHub [Online]. https://github.com/eucall-software/simex_platform [2016].