XFEL Operations Scheduling Guideline

This document discusses the impact, and consequent limitations, some operation parameters requested (needed) by specific experiments at a scientific instrument and thus a specific FEL source have to the flexibility, interference and performance of the other FEL sources. In order to avoid/reduce these impacts, the scheduling of activities (experiments) at the different FEL sources needs to be optimized. This document attempts to provide an overview of such constraints and suggests specific restrictions in order to minimize the interference

The most important parameter in this regard are the achievable photon energy ranges for the FEL sources. The photon energy generally depends on the electron beam energy and the magnetic gap. Since we operate the electron accelerator at only one electron energy at the time, there is a strict connection between the possible photon energies for soft and hard X-rays. For each electron energy the variable magnetic gap allows a certain photon energy range to be attained (see Fig. 1 and Annex figures). However, the magnetic value is not a 'fully free' parameter. The further the gap is opened, the less is the magnetic field and the less is the control of the SASE process. In addition, the magnetic phase error is only compensated up to a certain max. gap value (20 mm for SA1/2; 25 mm for SA3) i.e., the operation gap range of the respective undulator system. It is for these reasons that the difficulty of achieving good lasing conditions and thus reaching high FEL performance (stability, pulse energy) is increasing with magnetic gap value (compare Fig. 1).

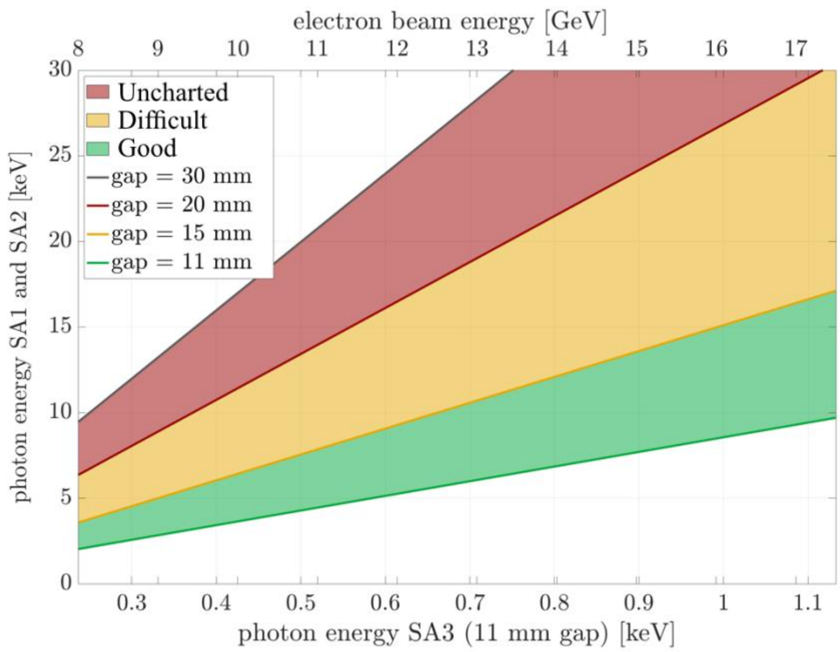


Figure 1: Photon energy range attainable at SA1/2 as a function of the SA3 photon energy.
The later corresponds to a specific electron energy, assuming a magnetic gap of 11 mm.
The colour code of the performance areas is explained in the text.

To provide guidance about how the electron energy and gap dependence affects the performance of the hard X-ray FELs SA1/SA2 we have created the performance plot in figure 1. The plot shows three areas of performance: good, difficult, uncharted related to the magnetic gap value. For the smallest gap values 11 - 15 mm we consider it straightforward to achieve good lasing conditions/performance. Tuning to reach these conditions is reduced. This good performance offers the highest flexibility to operate the SA1/2 FELs in SASE and Non-Standard Operation Modes (see appendix) without further restrictions, or to achieve good performance if the SA3 FEL source is operated with Non-Standard Operation Modes. For gap values 15 – 20 mm operations becomes already more complex, even for SASE setups, and we thus consider here a moderate performance (reduced pulse energies and shot-to-shot stability). Operating SA1/2 in this regime significantly limits the possibility for using Non-Standard Operation Modes, both at SA1/2 and at SA3. Operating SA1/2 at gap values 20 – 30 mm is presently very difficult, requires significant tuning times, achieves only limited pulse energies at reduced stability, and excludes the use of Non-Standard Operation Modes. Any request to operate in this regime must be carefully prepared and risks must be assessed on a case-by-case basis.

In the following we provide a couple of specific guidelines for the scheduling, or even further, the use of the allocated X-ray Delivery Time. In the first section, some general aspects are listed that should be considered when scheduling different experiments to be performed during the same period (typically a week). In the second section, comments for specific Non-Standard Operation Modes or parameter requests are listed. No particular order of these lists is intended.

General aspects for scheduling

- Frequent changes of delivery parameters (e.g. photon energies or intra bunch train repetition rates) potentially impact the performance of the other FELs sources. This interference effect is in particular observed for the SA1 and SA3 FELs. Most influences can be compensated for by downstream feedbacks, but these corrections are not instantaneous and thus lead to a reduction of X-ray time with regular performance.
- Additional tuning shifts may be needed in weeks with requests for Non-Standard Operation Modes (see appendix) or hard X-ray parameters outside the Good Zone. This will be decided on a case-by-case basis by the OB.
- Hard X-ray photon energies above the Good Zone area should preferably be scheduled in the last weeks of a given electron beam energy. This would allow the accelerator operators to further improve the performance of the facility week by week, while delivering FEL beams with less demanding parameters.
- If 4.5 MHz operation is scheduled, all instruments should schedule experiments taking advantage of the high repetition rate, and operate at least at 1 MHz. Running with lower repetition rates will increase the power load in the TLD dump and can, besides violating the ALARA principle, lead to problems with operation of the dump beamline.

Special aspects of Non-Standard Operation Modes

- **Scheduling Non-Standard Operation Modes:** It should be avoided to schedule two experiments with different parameters[1] in one week at the respective instrument requesting a Non-Standard Mode. Additional tuning time is likely required for these modes, which reduces the already limited time of at least one of the experiments.
- **Dedicated short pulse modes in SASE1 or SASE3:** In this case we need to operate SA1 and SA3 with a non-interleaved delivery pattern in order to allow individual compression setups for both FELs.

[1] If at least one of the following applies: 1. Most influences can be compensated for by downstream feedback, but this correction cannot be instantaneous. 2. Photon energy difference larger than 1 keV for a HXRSS setup. 3. Change of HRXSS priorities (e.g. background subtraction important or not). 4. Photon energy changes larger than 1 keV with split undulator setups.

- **Operation of SASE3 at gaps large 18 mm**: In cases where SA3 operates at photon energies at the upper end of the respective photon energy range for a given electron energy and is given a priority, the respective SASE1 experiments for this week should stick to a unique photon energy, intra bunch train repetition rate, and number of bunches. Only this avoids that SA3 will experience changes of the SA3 FEL properties related to parameters changes in SA1. The feasibility of requested SASE1 parameter changes with mitigation of SA3 property changes will be judged on a case-by-case basis.
- **Rolling pulse patterns** (changing bunch number and/or bunch positions from train to train in at least one beamline): If one Instrument uses this Non-Standard Mode, the other FELs should run with constant intra bunch train repetition rates. For the rolling pulse pattern mode, so called meta-patterns are used, including the bunch patterns of all FELs. A change in repetition rate in any of the FELs thus has the consequence that all meta-patterns of the rolling pulse pattern have to be adjusted.
- **Full bunch train on demand in one beamline.** The RF parameters have to be the same for all beamlines. This leads to an impact on highest achievable pulse energies and shot-to-shot stability.
- **Experiments with high sensitivity on background radiation[2] in SA1 and SA3:** In these cases, the other FEL/instrument should not be allowed to request long bunch trains as this will lead to an increase of the background.
- **Scheduled changes in SASE1 day and night**: During weeks of demanding or difficult performance (compare Fig. 1) or in case the priority experiment (day) is using a Non-Standard Operation Mode, the night experiment should, in general, not request changes of the X-ray delivery parameters. The limited tuning time at the beginning of the week will be fully dedicated to the priority experiment, and thus no preparation for a different operation setting during nights is possible. No experts will be available outside normal working hours and no additional tuning will be possible after switchover for the nightshift, because this would interfere with SASE3 operation. Furthermore, it is necessary that the setup for the leading experiment can be recovered in the morning. On a case-by-case basis, changes of the bunch-patterns might be possible (considering the impact on SASE3 operation) and small variations[3] of the photon energy are not judged as a problem.

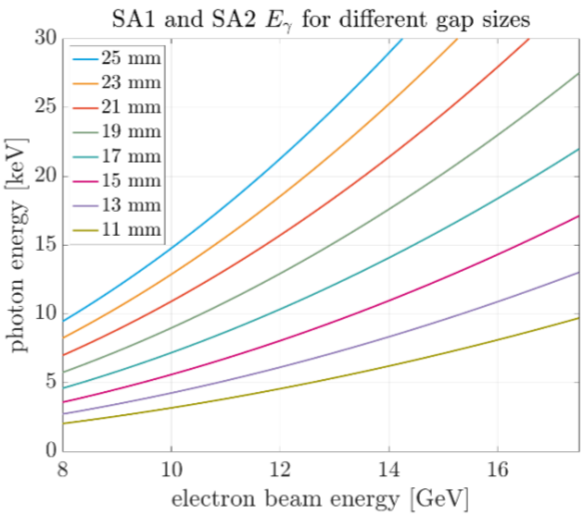
[2] By background radiation we mean here the spontaneous undulator radiation of the bunches that are dedicated for the other beamline. This is especially true if the sample can be damaged by the background radiation. Detector saturation can be avoided by moving the bunches of the respective experiment to the end of the pulse train and starting data acquisition just in time.

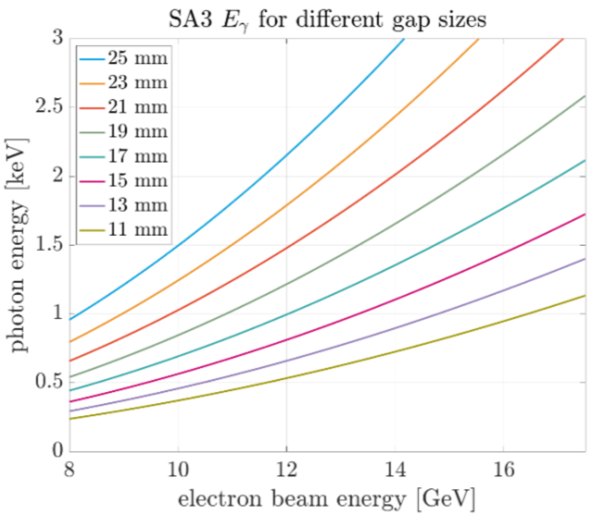
[3] Small variations of photon energy are considered +- 2 keV if operating in the good performance area.

Appendix

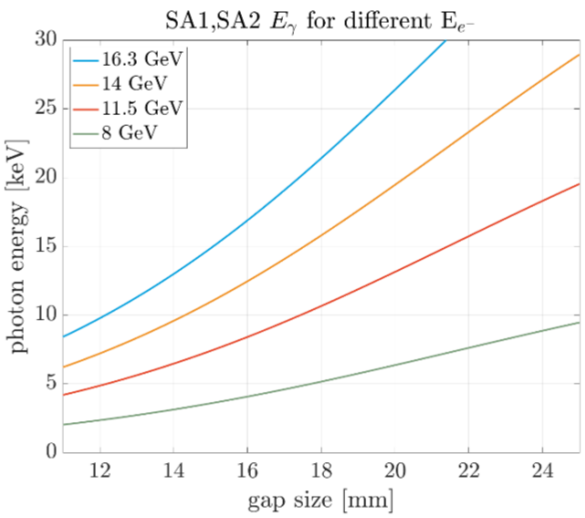
Photon energy ranges

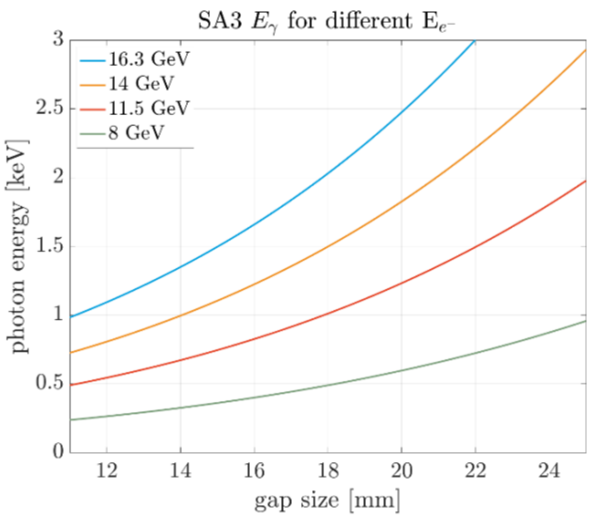
The following plots shows the resulting photon energies in the hard X-ray and soft X-ray undulator beamlines for given electron beam energies and for a selection of undulator gap sizes.





The next plots show comparable data, again for both undulator types, but with a different focus. They present the resulting photon energy for the four typical electron beam energies for different gap sizes of the undulators.





Non-Standard Operation Modes SASE1

Performance	Constraints	Additional Tuning Time	Available Techniques	Comments
Short pulses: < 10 fs	Non-interleaved	1 Shift	Non-linear compression, possibly with variable charge Wakefield-based short pulses	
	Reduced intensity compared to non-interleaved mode	1 Shift	Variable charge	
2 Colors: > 100 uJ/pulse	<10 keV (requires 14+ GeV) • Pulse length of maximal 30fs for each color • No controllable delay • Minimal color separation of 50 eV	1 Shift	Split undulator	All HXR split undulator experiments have been performed at SA2. However, we are confident that we can also deliver 2 Pulses at SA1.

Non-Standard Operation Modes SASE2

Performance	Constraints	Additional Tuning Time	Available Techniques	Comments
Short pulses: < 5 fs		1 Shift	Non-linear compression Chirp/Dispersion/ Compression	Likely well below 5 fs in the most extreme cases
2 Colors: > 100 uJ/pulse	<10 keV (requires 14+ GeV) • Pulse length of maximal 30fs for each color • Delay between 5fs and 300 fs (temporal pulse overlapping possible with a minimal color separation of 50 eV) • No zero-delay-crossing	1 Shift	Split undulator	
Spec. density: BW ~1eV FWHM 400-700uJ in the seeded BW	6 - 10 keV	2 Shifts	HXRSS	Routine user delivery mode. We did experience some performance degradation lately. Up to 400 bunches/train with rep-rate up to 2.25MHz with some decay in intensity along the pulse train. **6-8 keV temporarily restricted to 10 Hz due to broken equipment. More pulses per train will likely lead to a shift of both central wavelength and bandwidth along the pulse train.**
Spec. density: BW ~1eV FWHM 200-400uJ in the seeded BW	10 - 14 keV			

Non-Standard Operation Modes SASE3

Performance	Constraints	Additional Tuning Time	Available Techniques	Comments
Short pulses: < 5 fs >500 uJ	Non-interleaved	1 Shift	Chirp/Dispersion/Compression potentially coupled with variable charge	Delivered several times. In most extreme cases down to single spikes.
Short pulses: < 10 fs	Reduced intensity compared to non-interleaved mode	1 Shift	Variable charge	
2 Colors: <1 keV: >400 uJ/pulse 1 - 1.5 keV: >200 uJ/pulse 1.5-2 keV: >100 uJ/pulse	• Pulse length of maximal 30fs for each color. • Delay between 50fs and 500 fs (temporal pulse overlapping possible with a minimal color separation of 50 eV). No zero-delay-crossing	1 Shift	Split undulator	Delivered several times.
2 Colors & Short Pulses:	Non-interleaved	2 Shifts	Chirp/Dispersion/Compression Split undulator	Requires expert involvement