A hard X-ray self-amplified spontaneous emission free-electron laser optimization using evolutionary algorithms for dedicated user applications

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Abstract: Accelerator-based fourth-generation light sources are utilized in a wide range of interdisciplinary applications such as nanotechnology, materials science, biosciences, and medicine. A hard X-ray free-electron laser (FEL), as a state-of-the-art light source, was optimized using evolutionary algorithms for dedicated user applications such as X-ray Raman scattering (XRS), resonant inelastic X-ray scattering (RIXS), and X-ray emission spectroscopies (XES). Optimal parameter sets were obtained for an in-vacuum planar undulator driven by an 8 GeV electron beam. Performance parameters of self-amplified spontaneous emission (SASE) operation (i.e. optimized SASE performance parameters through evolutionary algorithms) were found to be consistent with operating X-ray FEL facilities around the world. It is shown that FEL characteristics for specific user experiments can be optimized by finding several evolutionary algorithm solutions within the range of 5 keV to 10 keV.

Key words: X-ray free-electron laser, undulator, evolutionary algorithms, optimization, inelastic X-ray scattering

1. Introduction

The unprecedented beam properties provided by X-ray free-electron laser (XFELs) have paved the way for the ultrasmall, ultrafast world [1,2]. XFEL radiation makes it possible to track the dynamics of chemical processes by taking snapshots of the motion of atoms, molecules, and clusters on an ultrafast timescale with atomic resolution. It offers the possibility of investigating samples that are sensitive to radiation damage, weakly scattering samples, and time-resolved processes that are irreversible. Radiation damage is one of the main challenges in determining the structure of proteins that cannot be crystallized. Using ultrafast and intense pulses, the structure can be determined by X-ray scattering in a single shot before radiation damage occurs [3]. X-ray pulses with a large number of photons can be focused on a spot that is approximately the size of a virus or the smallest structures fabricated on an electronic chip. XFEL radiation exhibits unprecedented coherence, which enables us to explore new domains of dynamical processes [1,2]. By pooling the energy of coherent photons, multiphoton excitations can be created and various nonlinear X-ray experiments can be performed, which is a largely unexplored area of science. XFELs also provide unique possibilities for the generation and diagnosis of dense, strongly coupled plasmas as well as warm dense matter research [4,5].

Unique features of XFELs are utilized in different user experiments conducted over a broad spectral region ranging from ultraviolet to hard X-rays. Using extremely intense and short X-ray pulses of XFEL, femtosecond

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time resolution inelastic X-ray scattering (IXS) experiments can be performed to investigate the electronic and structural dynamics of a wide range of systems [6]. Nonresonant inelastic X-ray scattering (NRIXS), also known as XRS, is a synchrotron-based technique used for the investigation of low-energy absorption edges of elements such as C K-, Fe L-, or La N- edges (50 eV to 1000 eV) using hard X-rays (approx. 10 keV) [7]. Providing bulk-sensitive probes and not requiring vacuum conditions, it is preferred to conventional soft X-ray absorption spectroscopy (XAS) measurements (below 1 keV) for complicated sample environments such as diamond anvil cells [8], liquids [9], or samples under in situ conditions [10]. In the XRS technique with synchrotron sources, the incoming photon energy is usually scanned as the scattered photons are measured at fixed energy. The performance of synchrotron-based X-ray spectroscopy techniques may differ in the use of XFEL radiation. When the XRS technique is conducted with XFEL sources, a dispersive hard X-ray spectrometer operating at a fixed incident beam energy is used. Dispersive IXS spectrometers based on von Hamos geometry consist of cylindrically bent multicrystal analyzers to simultaneously energy-resolve the broad spectral range of the X-rays scattered or emitted by the sample [11–13]. The geometry makes it possible to measure the spectrum in a single shot, without scanning any part of the spectrometer or the incident beam energy. The compact and portable spectrometer can operate in the 5 keV to 10 keV region and be used for both off- and on-resonant X-ray techniques such as XRS, XES, and RIXS [6] at XFEL and synchrotron radiation facilities for time-resolved applications such as pump-probe measurements [11–13]. Combining a dispersive IXS spectrometer with femtosecond XFEL pulses enables to study ultrafast electronic structure dynamics in diluted samples, biological samples sensitive to radiation damage, and samples under high pressure/high temperature or in situ conditions.

Combinatorial optimization problems [14] that involve finding optimal parameter sets from a large search space [15] can be solved using heuristic approaches such as multiple objective evolutionary algorithms (MOEAs). MOEAs, which are essentially stochastic search methods, are used to reduce the complexity of the problem, unlike finite element simulations or analytical methods [16]. Identification of the optimal parameters for a physical design problem [17] (i.e. finding optimal parameters for hard X-ray FEL operations for specific applications) is investigated in this study using NSGAIII [18] for its ability to generate uniformly distributed solutions in the search space.

The purpose of the study is to find the best performance parameters for self-amplified spontaneous emission (SASE) operation utilizing evolutionary algorithms. FEL characteristics for dedicated user experiments (e.g., XRS, RIXS, and XES) can entirely be optimized through evolutionary algorithm solutions from 5 keV to 10 keV photon energies. Since the quality of FEL pulses is directly based on the undulator magnetic structure and electron bunch characteristics, numerous entangled parameters have to be carefully optimized. In this respect, the main performance parameters of SASE operation (i.e. saturation power, Pierce parameter, saturation length) were thoroughly optimized via genetic algorithms.

2. Optimization of SASE operation

In order to achieve the photon energy range from 5 keV ($\sim$2.48 Å) to 10 keV ($\sim$1.24 Å) using MOEAs, the problem is represented as a simple chromosome comprising two genes for the undulator period (λ_u) and undulator gap (g). Since this is a continuous optimization problem, a real-valued representation [19] for the chromosome structure was used. The optimization problem in this study has two main goals (G1 and G2). The first goal is to improve the FEL power denoted by P_{sat} and the second goal is to achieve λ_{FEL} down to

sub-angstroms. These goals are defined in Eqs. 1 and 2:

$$G_1 = P_{sat} \tag{1}$$

and

$$G_2 = 1.0/\lambda_{FEL}, \tag{2}$$

subject to the conditions shown with C_i:

$$C_1 = 0.1 \leq g/\lambda_u \leq 1.0,$$
$$2\ mm \leq g \leq 80\ mm, \tag{3}$$
$$15\ mm \leq \lambda_u \leq 40\ mm,$$

$$C_2 = 1.0\ \text{Å} \leq \lambda_{FEL} \leq 2.5\ \text{Å}, \tag{4}$$

$$C_3 = 50\ m \leq L_{sat} \leq 250\ m, \tag{5}$$

where P_{sat} in Eq. 6 is the saturation power, λ_{FEL} in Eq. 7 is the wavelength of the laser, and L_{sat} in Eq. 8 stands for the saturation length [20,21]:

$$P_{sat} \approx \rho P_{beam}^{peak} = 1.6\rho(L_{G,1D}/L_{G,3D})^2 P_{beam}^{peak}, \tag{6}$$

$$\lambda_{FEL} = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2}\right), \tag{7}$$

$$L_{sat} = L_{G,3D}\, ln\left(\frac{9\lambda_{FEL}P_{sat}}{\rho^2 c E_{beam}}\right). \tag{8}$$

3. Results and discussion

A hard X-ray free-electron laser was optimized for dedicated user experiments such as XRS, RIXS, and XES. Since the compact and portable spectrometer mentioned above can operate in the energy range of 5–10 keV, crucial performance parameters for SASE operation are estimated by using evolutionary algorithms. Figure 1 shows that a high-power X-ray FEL in the 5 keV to 10 keV photon energy range can be generated with some GWs of saturation power. On the other hand, Figure 2 displays that SASE operation enables plausible Pierce parameter values for the dedicated wavelength range. Finally, the novelty of this study is that an 8 GeV electron beam is sufficient to generate hard X-ray FEL pulses by means of a hybrid with Vanadium Permendur planar undulators [21].

4. Conclusion

X-ray FELs, combining the unique properties of FEL radiation with atomic resolution as well as penetration power offered by X-rays, provide high-tech applications for interdisciplinary scientific research. Unprecedented properties of XFELs are utilized in soft and hard X-ray regimes for different user experiments. The dispersive IXS spectrometer operating with femtosecond X-ray pulses in the energy range of 5 keV to 10 keV provides investigation of ultrafast electronic structure dynamics in complex sample environments. In this study, it is
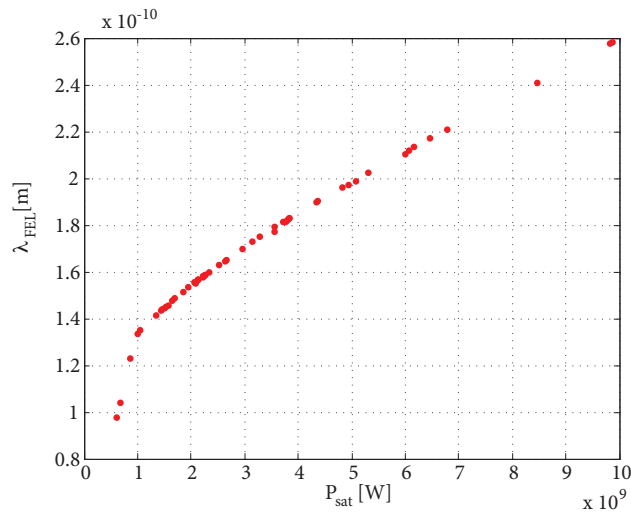
Figure 1. Pareto optimal solutions for λ_{FEL} vs. P_{sat}. Note that each data point corresponds to an individual solution obtained through the evolutionary algorithm and should not be interpreted as a function of the axes.

Figure 2. Pareto optimal solutions for λ_{FEL} vs. Pierce parameter (ρ). Note that each data point corresponds to an individual solution obtained through the evolutionary algorithm and should not be interpreted as a function of the axes.
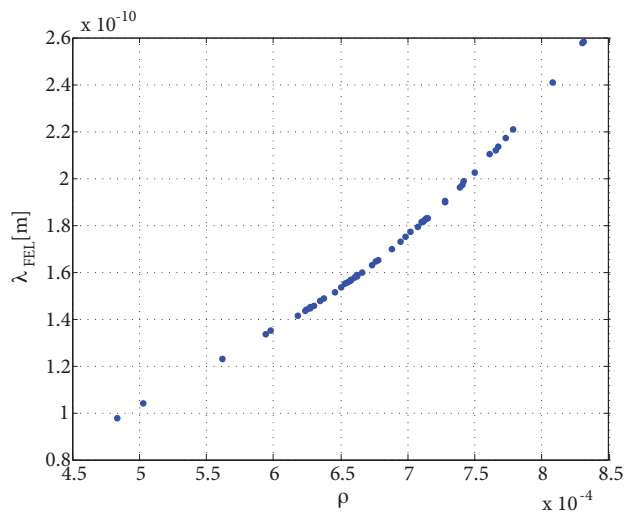
shown that FEL characteristics for dedicated user experiments such as XRS, RIXS, and XES can thoroughly be optimized by various evolutionary algorithms solutions from 2.48 Å down to 1.24 Å. As a result, optimal parameter sets for an 8 GeV linac-driven planar in-vacuum undulator were obtained and found to be consistent with the operating X-ray FEL facilities worldwide.

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