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# Multi-dimensional optimization of a terawatt seeded tapered Free Electron Laser with a Multi-Objective Genetic Algorithm

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## ABSTRACT

There is a great interest in generating high-power hard X-ray Free Electron Laser (FEL) in the terawatt (TW) level that can enable coherent diffraction imaging of complex molecules like proteins and probe fundamental high-field physics. A feasibility study of producing such X-ray pulses was carried out employing a configuration beginning with a Self-Amplified Spontaneous Emission FEL, followed by a “self-seeding” crystal monochromator generating a fully coherent seed, and finishing with a long tapered undulator where the coherent seed recombines with the electron bunch and is amplified to high power. The undulator tapering profile, the phase advance in the undulator break sections, the quadrupole focusing strength, etc. are parameters to be optimized. A Genetic Algorithm (GA) is adopted for this multi-dimensional optimization. Concrete examples are given for LINAC Coherent Light Source (LCLS) and LCLS-II-type systems. Analytical estimate is also developed to cross check the simulation and optimization results as a quick and complimentary tool.

## 1. Introduction

Single molecule imaging and in general the study of structures on the nanometer or even finer level requires more than $10^{13}$ hard x-ray photon/second in a pulse within femtosecond duration [1–4]. This calls for a Free Electron Laser (FEL) having high power of the order of terawatts (TW). A promising approach to reach TW powers is to increase the energy transfer from the electrons to radiation by adjusting the undulator magnetic field to compensate for the electron energy losses or tapering the undulator [5]. During the FEL process, the electrons keep losing energy and eventually the electron bunch centroid energy becomes so low that it no longer satisfies the resonant condition determined by the initial electron bunch centroid energy. Hence, one has to gradually reduce the undulator strength so that the resonant condition determined by the initial electron bunch centroid energy is being maintained. However, a previous study has shown that simply tapering the undulator for a FEL working in the Self-Amplified Spontaneous Emission (SASE) mode is not sufficient to reach TW power [6]. A seeded FEL responds more efficiently to the tapered undulator [7] and can potentially bring the FEL to TW level. A proof-of-concept design for TW FEL based on self-seeding [8,9] and tapering scheme has been developed for European XFEL [10,11], the future MAX IV FEL [12] as well as for LINAC Coherent Light Source (LCLS)/LCLS-II [13,14] with LCLS-type electron bunch [15] and LCLS-II-type variable gap undulator [16], or even superconducting undulator [17]. More general studies on tapered FELs are reported [18,19].

As is well known and experimentally verified, for an undulator with constant strength $K$, high gain single pass FEL amplifiers reach saturation at a power level of $P_{\text{sat.}} \sim \rho P_{\text{beam}}$ where $P_{\text{beam}}$ is the electron beam power and $\rho$ is the FEL efficiency parameter [20,21], which is normally smaller than 0.1% for hard X-ray FEL. This behavior is true for both SASE and externally seeded configurations. This saturation arises from the growth of slice energy spread and the rotation of the microbunched electrons in the ponderomotive potential well, which is

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formed by the FEL radiation and the undulator magnetic field. For electron beam parameters corresponding to the proposed LCLS-II project at SLAC National Accelerator Laboratory, $\rho \sim 5 \times 10^{-4}$, the nominal saturation power is ~30 gigawatts (GW), far below the TW level. However, near and at exponential growth saturation point the microbunching fraction is large (bunching factor: $b_1 \sim 0.5$), suggesting that with proper tapering of the undulator strength $K$, one can both trap and then decelerate a considerable fraction of the electrons to extract much greater additional power [5]. For example, currently LCLS doubles its output power to ~70 GW using its very limited available tapering range of $\Delta K/K \sim 0.8\%$. While for the examples shown below, for a seeded tapered FEL, the extraction efficiency defined as $\eta \equiv P_{\mathrm{FEL}}/P_{\mathrm{beam}}$, can go well above 1%, so that the FEL power can go above 1 TW, making the single molecular imaging close to reality. Such high-field FEL also opens the possibility to study physics at the Schwinger Limit. Without the taper, the extraction efficiency $\eta = \rho$, the FEL efficiency parameter.

The proposed LCLS-II undulators have fully tunable gaps and thus in principle can taper $K$ to zero. Moreover, there is currently a great interest in giving LCLS-II a self-seeding option employing the crystal monochromator scheme [8]. Consequently, as shown in Fig. 1, a TW-level FEL starts with a SASE undulator (the first part of the undulator system) having a sufficient length to generate GW-level radiation. This radiation then passes through a crystal monochromator that results in a megawatt (MW)-level, nearly monochromatic wake, which will seed the electron bunch in the downstream undulator (the second part of the undulator system). In the LCLS case, one utilizes the Bragg forward deflection part of the SASE FEL [8,9]. During the time when the radiation passes through the monochromator, the electron bunch is deflected in a by-pass magnetic device, called a chicane. The chicane is tuned so that the electron bunch is time-delayed and rejoins the coherent seed (the monochromatic wake). The coherent seed and the electron bunch then enter the second part of the undulator system in which the coherent seed first grows exponentially to saturation. Then, by tapering the undulator strength $K$ to maintain the resonance condition defined in the exponential growth process, a highly micro-bunched electron bunch continually amplifies the radiation, which can strongly grow to TW power level [13]. The growth of the radiation power in the tapered region is almost linear. This linear growth will eventually stop due to electrons de-trapping from the ponderomotive potential well [14]. The de-trapping phenomenon happens due to various reasons, such as the three-dimensional effect, the side-band instability, the temporal non-uniformity, etc.

Properly setting the tapered undulator strength is crucial to maximizing the FEL radiation power. Because the coherent emission is strongly dependent on the capturing ratio of the electrons by the ponderomotive buckets which in turn depends on the history of the interaction between the electron bunch and the radiation field, optimizing the tapering profile is a complicated problem that needs to take into account both the longitudinal and transverse coupling between the electrons and the radiation field. The main concern of this optimization problem is whether the global optimum can be found. In Ref. [14], an iterative 1-dimensional parameter scan method is used for this optimization problem with a model of 8 variables. In this study we extend both the tapering model and the transverse focusing model to higher orders and also experiment with phase shifter variations, which makes the optimization problem more complex. We adopt a new optimization method called Multi-Objective Genetic Algorithm (MOGA) which has recently found applications in the accelerator and beam physics field [22–28]. Application of the MOGA method to optimizing a TW FEL is a novel approach in FEL studies. This method has allowed us to explore the parameter space more thoroughly and given us better assurance to the optimal solution.

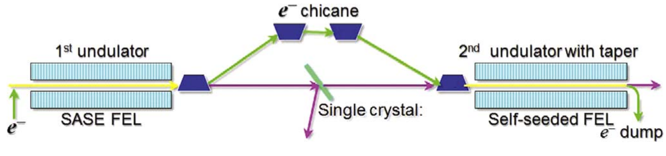

**Fig. 1.** Schematic of a TW FEL starting with a SASE FEL, followed by a "self-seeding" crystal monochromator, and finishing with a tapered undulator.

The paper is organized as follows. In Section 2, we extend the taper physics model as compared to that in Ref. [13,14] to include high-order terms. We also study the role of phase shifters in the undulator break sections. The variables as well as the objectives are explained. The Multi-Objective Genetic Algorithms (MOGA) is described in Section 3 with a brief review of grid-scan type optimization as in Ref. [14]. To illustrate some of the key physics behind this complicated optimization, we present an analytical estimate of the taper profile in Section 4 to reveal the scaling on various parameters as well as to cross check the numerical results as far as possible. Results and Discussions are presented in Section 5. A brief conclusion is in Section 6.

## 2. LCLS-II taper models and optimization

We have developed an approach [14] to empirically optimize $K(z)$ tapers together with the external-focusing strength superimposed on the undulator sections to maximize the output power at a fixed total undulator length. In Refs. [13,14], we proposed to formulate the taper as a mathematical function

$$K(z) = K_0\left[1 - a\left(\frac{z - z_0}{L_w - z_0}\right)^b\right], \tag{1}$$

where $z$ is the position coordinate along the undulator system, $K_0$ the initial undulator strength, $z_0$ the location where the undulator starts to be tapered, $L_w$ the undulator length, $a$ the fractional tapering at the end of undulator, i.e., at $z = L_w$, and $b$ the taper changing rate which is not necessarily an integer. As explained in Section 4, $b$ is close to 2, i.e., a quadratic taper. We further explore the taper model by adding higher-order terms. The contribution from the high-order terms is elaborated in Section 5.

The external-focusing strength optimization results in a $z$-dependent electron beam transverse size for better coupling to the radiation mode size. In our study, the external focusing is realized by an alternating strong-focusing quadrupole lattice. We introduce a three-segment variation of the electron bunch transverse size $r_b$ by changing the quadrupole field strength $K_q(z)$ with $z$:

$$K_q(z) = \begin{cases} K_{q0}, & 0 \le z \le z_1 \\ K_q(z_1)[1 - f(z - z_1)^n], \quad \text{for} & z_1 < z \le z_2 \\ K_q(z_2)[1 - g(z - z_2)^n], & z_2 < z \le L_w \end{cases}, \tag{2}$$

where $n$=1 or 2, $z_1$ indicates the starting point of $K_q$-variation, which is usually around the end of the exponential growth regime; $z_2$ indicates the starting point of the third segment; $f$ can be either positive or negative, while $g$ is usually negative. In Refs. [13,14], we set $n$=1, and gave a detailed description of the physics behind it. As what will be explained later, due to the coherent emission, the radiation power is higher for an electron bunch with smaller transverse size, but on the other hand, a smaller electron bunch leads to larger diffraction. A strong focusing is normally favored in the simulation, hence a scaling stronger than linear is studied in this paper with $n$=2 as well.

As explained above, in Refs. [13,14], the optimization was done in 8-dimensional space with one objective with a grid-scan type of algorithm, i.e., $a$, $b$, and $z_0$ in Eq. (1), and $K_{qO}$, $f$, $g$, $z_1$, and $z_2$ in Eq. (2). However, using a single objective function based on final radiation power may not be sufficient in practical applications since other higher order transverse modes besides the fundamental Gaussian mode can also contribute to the radiation power [29]. To evaluate the quality of radiation, we define another objective function, the radiation pseudo-