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Optimization of SASE operation for an X-ray free-electron laser Using multiple objective evolutionary algorithms

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Performance of Self Amplifed Spontaneous Emission (SASE) operation for an X-ray Free-Electron Laser (FEL), is optimized by Multiple Objective Evolutionary Algorithms (MOEA). Different types of hybrid planar undulators are considered to achieve 0.5 Å ≤ λ_{FEL} ≤ 1.5 Å wavelength range. This demand is regarded as a continuous optimization problem, and hence, an evolutionary algorithm is designed to find optimal FEL performance parameters. An encoding scheme comprising of undulator period (λ_u) and undulator gap (g) is adopted here to find optimal values for saturation power (P_{sat}) and λ_{FEL} subject to several physical constraints on λ_u and g such as the ratio of g/λ_u and L_{sat}. It is shown that MOEA gives optimal solutions for estimation of L_{sat} with plausible P_{sat} values.

Keywords: Undulator, X-ray free-electron laser, Self amplified spontaneous emission, Multiple objective evolutionary algorithms, Linear accelerator

1 Introduction

Accelerator-based fourth generation light sources, namely FELs, provide high power, monochromatic, coherent, tunable and ultra-short pulses[1,2,3]. Leading X-ray FEL facilities around the world (*e.g.* European XFEL[4], LCLS[5], FLASH[6], SACLA[7] etc.) are based on state-of-the-art linear accelerator (linac) and undulator technologies. Since no 'X-ray reflecting mirror' is available in today's technology, FEL-oscillators are unserviceable for X-ray FEL generation. Hence, single pass SASE operation without any mirrors is the only way for generation of X-ray FELs via sequential array of undulators along a linear path. The undulator is a device which simply consists of two long rows of alternating dipole magnets. When bunches of electrons running almost at the speed of light enter to the undulator line, magnetic forces cause them to oscillate. This constant change in velocity lead electrons to emit X-rays. Afterwards, expended electron bunches are forwarded to the beam dump.

Evolutionary algorithms[8] including genetic algorithms, genetic programming and evolution strategies have received a considerable amount of attention for their proven success in the optimization of complex functions[9,10,11] frequently tackled in engineering problems. Researchers have used unimodal and multimodal complex functions as benchmarks to show the potential of such algorithms. These algorithms create an initial population with candidate solutions for the optimization problem and then use genetic operators such as selection, recombination and mutation in order to create new solutions and test whether these new solutions are approaching towards the optimal solution[12]. The objective function, *i.e.* the fitness function, used here in order to evaluate the quality of each newly generated solution.

The main strength of evolutionary algorithms here is the ability to define criteria to eliminate unfeasible solutions using penalty schemes[13]. This makes it possible to incorporate physical requirements or constraints such as expecting the ratio $0.1 < g/\lambda_u < 1$ or the value of the λ_{FEL} around sub-Angstroms. In the design of the evolutionary algorithm so that the optimal solutions found by the algorithm are in line with physical rules. This is elaborated in Section 3.3.

This paper presents the use of evolutionary algorithms[14] in order to achieve 0.5 Å ≤ λ_{FEL} ≤ 1.5 Å for SASE operation. The problem is encoded in a suitable model and then an evolutionary search was performed over generations using multiple objective evoluationary algorithms (MOEA) namely: NSGA (Non-dominated Sorting Genetic Algorithm)[15], GDE3 (Generalized Diferential Evolution)[16,17] and

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ϵ-MOEA[18]. The main objectives of this optimization problem are two-fold: The first objective is to enhance the power of the laser (P_{sat}) and the second one is to lower wavelength (λ_{FEL}) down to hard X-rays. Pareto optimal solutions[19] found by these algorithms are demonstrated along with a discussion of how these solutions can be interpreted. Therefore the contributions of this paper are as follows:

- A hard X-ray free-electron laser is feasible *via* short-period in-vacuum undulators.
- A 8 GeV electron linear accelerator is sufficient to achieve 1 Å FEL wavelength.
- Hybrid with Vanadium Permendur and Hybrid with iron undulators are employed.
- Self Amplifed Spontaneous Emission (SASE) operation is utilized for lasing process.
- FEL parameters are optimized using multiple objective evolutionary algorithms.

The rest of the paper is organized as follows: Section 2 summarizes X-ray undulators followed by Section 3, where the evoluationary algorithm based parameter optimization method is explained. Section 4 presents and discusses findings. Finally, the paper is concluded in Section 5.

2 X-ray Undulators and SASE Principle

Regarding design issues, planar or helical undulators are employed depending on users' requirements such as: linear or circular polarized photon pulses. Although mechanical tuning of helical devices are relatively hard and complicated, generation of circular-polarized photons within shorter gain lengths may be desirable for dedicated FEL facilities[3].

In addition, most of the user experiments require linear polarized photon pulses. Here below, generation of an FEL pulse by SASE principle, whereby a relativistic electron moves along a sinusoidal path resulting in radiation with a number of electromagnetic waves equivalent to number of undulator periods, is evaluated. This radiation has a narrow bandwidth which is inversely proportional to the number of undulator periods[20].

Considering a bunch of 10^9-10^{10} electrons travelling along an undulator line, the emitted radiation is the sum of electromagnetic fields generated by them. Eventually the amplitude increases exponentially with a growth rate called "gain length"[20]. As soon as all electrons are well-synchronized, exponential growth reaches saturation (see Eq. 1)[21].

$$P = \alpha P_n e^{z/L_g} < P_{sat} \quad \text{... (1)}$$

As to the correlation between X-ray FEL pulses and electron bunches, a high quality electron beam undoubtedly generates high quality FEL pulses. Hence, in order to achieve high-grade X-ray photons, an advanced electron beam is essential as a matter of course. In this respect, transverse emittance (Eq. 2), peak current (Eq. 3) and peak power of the electron beam (Eq. 4) come into prominence. In Eq. 2, $\sigma_{x,y}$ and $\beta_{x,y}$ are transverse beam sizes and beta functions, respectively. Concerning the concept of normalized emittance ($\varepsilon_{x,y}^N$), which is a constant along the linac, is simply "γ-Lorentz factor" multiple of transverse emittance for a relativistic beam. In Eq. 3, Q is the bunch charge, where t_μ is FWHM (full width at half maximum) bunch length in time domain. As seen in Eq. 4, beam peak power (P_{beam}^{peak}) is calculated by multiplying the beam energy with peak current.

$$\varepsilon_{x,y} = \frac{\sigma_{x,y}^2}{\beta_{x,y}} \quad \text{... (2)}$$

$$I_{peak} = \frac{Q}{t_\mu} \quad \text{... (3)}$$

$$P_{beam}^{peak} = E_{beam} I_{peak} \quad \text{... (4)}$$

Regarding 0.5 Å ≤ λ_{FEL} ≤ 1.5 Å SASE FEL optimization, an 8 GeV electron beam (see Table 1) [22], is taken into account as a driver beam for hybrid planar undulators. In Table 1, it is the beam peak power which establishes saturation power of the FEL by Eq. 5. In other words, the higher the P_{beam}^{peak}, the higher the P_{sat}.

$$P_{sat} \approx \rho P_{beam}^{peak} = 1.6\rho\left(L_{G,1D}/L_{G,3D}\right)^2 P_{beam}^{peak} \quad \text{... (5)}$$

Table 1 — Parameters of an 8 GeV electron beam [22]

Beam energy, E_{beam}	8	GeV
Normalized emittance, $\varepsilon_{x,y}^N$	1	π mm.mrad
FWHM bunch length, t_μ	0.3	ps
Transverse beam sizes, $\sigma_{x,y}$	25	μm
Bunch charge, Q	1	nC
Peak current, I_{peak}	3.3	kA
Beam peak power	26.6	TW

On the other hand, as seen in Eqs. 6-8, two critical parameters, undulator period and gap, specify FEL wavelength for a dedicated electron beam energy.

$$\lambda_{FEL}\frac{\lambda_u}{2\gamma^2}\left(1+\frac{K^2}{2}\right) \quad ... (6)$$

$$B_{peak} = aExp\left[b\frac{g}{\lambda_u}+c\left(\frac{g}{\lambda_u}\right)^2\right] \quad ... (7)$$

$$K = 0.934\lambda_u[cm]B_{peak}[T] \quad ... (8)$$

In Eq. 9, the crucial performance parameter for SASE operation (Pierce parameter) is given[21], where $\xi = \frac{a_\omega^2}{2(1+a_\omega^2)}$ and $a_\omega = \frac{K}{\sqrt{2}}$ for a planar undulator. In addition, $J_0(\xi)$ and $J_1(\xi)$ are 0th and 1st order Bessel functions, respectively.

Finally, the constant of 17045 A is the Alfven current.

$$\rho = \left[\left(\frac{I_{peak}}{17045\ \mathrm{A}}\right)\left(\frac{\lambda_u a_\omega[J_0(\xi)-J_1(\xi)]}{2\pi\sigma_x}\right)^2\left(\frac{1}{2\gamma}\right)^3\right]^{1/3} \quad ... (9)$$

The 1D gain length ($L_{G,1D}$), which is an ideal case assuming that the electron beam has a uniform transverse spatial distribution with zero emittance and energy spread, is calculated by Eq. 10[21].

$$L_{G,1D} = \frac{\lambda_u}{4\pi\sqrt{3}\rho} \quad ... (10)$$

By using the universal scaling function (Eq. 11), $L_{G,3D}$ is obtained from $L_{G,1D}$ (see Eq. 12). In Eq. 11, η_d (a spatial 3D effect) is the gain reduction resulting from diffraction, where η_ε and η_γ are gain reductions on account of longitudinal velocity spread of the electron beam owing to emittance and energy spread[21].

$$\eta = 0.45\eta_d^{0.57} + 0.55\eta_\varepsilon^{1.6} + 3\eta_\gamma^2 + 0.35\eta_\varepsilon^{2.9}\eta_\gamma^{2.4} + 51\eta_d^{0.95}\eta_\gamma^3 + 5.4\eta_d^{0.7}\eta_\varepsilon^{1.9} + 1140\eta_d^{2.2}\eta_\varepsilon^{2.9}\eta_\gamma^{3.2} \quad ... (11)$$

$$\eta_d = \frac{L_{G,1D}}{L_R} \quad ... (12)$$

$$\eta_\varepsilon = \left(\frac{L_{G,1D}}{\beta}\right)\left(\frac{4\pi\varepsilon_t}{\lambda_{FEL}}\right) \quad ... (13)$$

$$\eta_\gamma = 4\pi\left(\frac{L_{G,1D}}{\lambda_u}\right)E_{spread} \quad ... (14)$$

$$L_{G,3D} = (1+\eta)L_{G,1D} \quad ... (15)$$

On the other hand, Rayleigh length of a laser beam is the distance from the beam waist where the beam radius attains $\sqrt{2}$-times longer in the propagation direction. In other words, concerning a circular beam, the area doubles itself along the Rayleigh range.

$$L_R = \frac{4\pi\sigma_x^2}{\lambda_{FEL}} \quad ... (16)$$

In order to determine the magnetic length of the undulator line, saturation length (see Eq. 17) has to be carefully optimized while keeping the saturation power in order of some GWs.

$$L_{sat} = L_{G,3D}ln\left(\frac{9\lambda_{FEL}P_{sat}}{\rho^2 cE_{beam}}\right) \quad ... (17)$$

3 Evolutionary Parameter Optimization

This section describes the evolutionary approach for finding optimal SASE parameters. In the following, first the general algorithm is discussed and then the application specific details are presented.

3.1. Algorithm

The approach is shown with its main stages in Fig. 1. The algorithm starts with an initialization stage where the population is filled with individuals which are candidate solutions to the optimization problem. Population is a collection of individuals with varying genotypes. Parameters to be optimized are randomly drawn from nominal ranges and assigned to individuals (candidate solutions) in the population. A fitness evaluation is performed here to decide on the parents for the recombination stage. In the recombination stage, new individuals (*i.e.* offspring) are generated and slight modifications to these new individuals in the mutation stage. A final fitness evaluation is performed for the new individuals and survivors are selected.

Following sections will elaborate on these stages of the evolutionary approach.

3.2. Encoding

Modeling the solutions to the real-world problem in form of chromosomes for the evolutionary

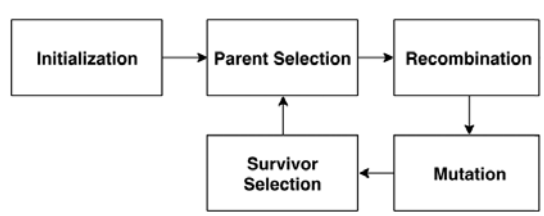

Fig. 1 — Evolutionary optimization cycle

algorithms is known as encoding or representation[23]. The representation is a two way encoding i.e. the candidate solution is encoded as a chromosome and a chromosome can be decoded back to the solution: from phenotype to genotype space and vice versa.

Here the problem is represented as a simple chromosome comprising of two genes for the undulator period (λ_u) and undulator gap (g). Due to the continuous nature of the problem, a real-valued representation[24] was employed in the chromosome structure.

3.3. Fitness function

The encoding of the problem requires a method for quantizing the quality of each candidate solution. The fitness function is used to evaluate the solutions and models the requirements that the individuals need to follow.

The physical constraints such as the expected range for the $0.1 < g/\lambda_u < 1$ and ρ being in the order of 10^{-4} is incorporated in the fitness as penalty terms[25] in order to penalize individuals yielding values that do not adhere to the constraints.

This optimization problem has two main goals (G1 and G2). The first goal is to improve the FEL power denoted with P_{sat} and the second goal is to achieve λ FEL down to sub-Angstroms. These goals are defined as:

$$G_1 = P_{sat} \quad \ldots (18)$$

and

$$G_2 = 1/\lambda_{FEL} \quad \ldots (19)$$

subject to conditions shown with C_i:

$$C1 = 0.1 \leq g/\lambda_u \leq 1,\ 2\text{mm} \leq g \leq 80\text{mm},\ 15\text{mm} \leq \lambda_u \leq 20\text{mm} \quad \ldots (20)$$

$$C2 = 0.5\text{Å} \leq \lambda_{FEL} \leq 1.5\text{Å} \quad \ldots . (21)$$

$$C3 = 50\text{m} \leq L_{sat} \leq 150\text{m} \quad \ldots (22)$$

3.4. Selection method

Deciding the subset of the population which will be used for the recombination and which will be used in the next generation is known as parent selection and survivor selection, respectively[26].

The former selection method creates a mating pool so that the recombination operators can generate new individuals using the existing parents. This methods aims to choose individuals (candidate solutions) with higher fitness levels so that high-quality genes can be transferred to subsequent generations. Selection is performed using a tournament selection[27]. In this selection method, tournaments of a specific size are created by filling the tournaments with individuals randomly selected from the population. The winning individual of each tournament is the one with the highest fitness value. The winners of the tournaments are collected in a mating pool, so that they will be picked randomly to engage in recombination phase.

The latter selection method decides the survivors of the population for the next generation[28]. The environment, solution space, is limited here so that only the fitter individuals can survive. Here, the individuals are simply sorted in descending order of the fitness and the ones with lowest fitness values are decimated according to the population size limit.

3.5. Genetic operators

Diversity of the population is critical to evolutionary algorithms[29] and it is important cover a significant portion of the search space with individuals having varying fitness values. This approach achieves this diversity by employing variation operator[12] so that the population can regenerate itself with new individuals with a general aim to maximise the fitness value. Genetic operators are examined in two groups considering the number of inputs they take [30], namely mutation and recombination:

Mutation. This unary operator applies small modifications on a single individual. The purpose of the mutation operator is to add individuals with newer genotypes to the population, improving diversity and hence exploring the unexplored locations in the search space. In this numeric optimization problem, genes in the chromosome are added with offset values of ±0.1 mm, selected randomly.

Recombination. This operator, also known as cross-over, is a binary operator which takes two individuals and create two new individuals to be added to the population. Recombination is the process where the genetic material of the parent genes are transferred to the offspring. The main principle behind this operator is that when two individuals with varying desirable features mate, it is likely that the offspring will posses both desirable features. Recombination is employed using whole-arithmetic recombination[31] for the encoding mentioned above. This simply computes a weighted average of the corresponding gene locations to generate two siblings:

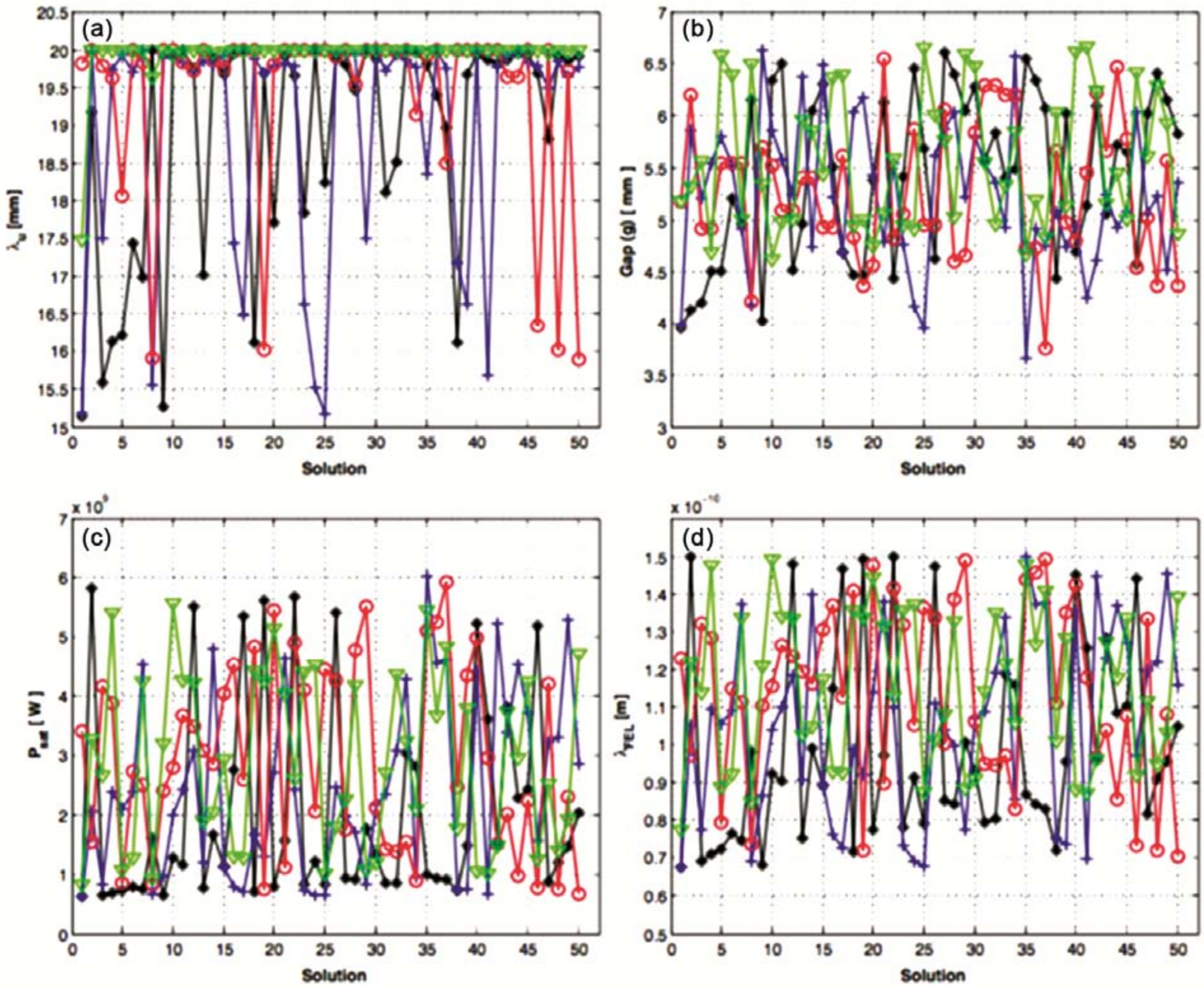

Fig. 2 — SASE performance parameters for hybrid with Vanadium Permendur (*) NSGAII, (+) NSGAIII, (o) GDE3 and (∇) ε-MOEA. (a) λ_u (b) g (c) P_{sat} (d) λ_{FEL}

$$c1 = \alpha \cdot p1 + (1-\alpha) \cdot p2 \quad \ldots (23)$$
$$c2 = \alpha \cdot p2 + (1-\alpha) \cdot p1$$

which uses α as the *aggregation weight* for combining alleles from both parents. Here α≠0.5, since this would generate two identical offspring.

It is worth mentioning here that the genetic operators aim to find global optima[32]. Both operators act differently on their approach to cover the search space, these strategies are known as exploration and exploitation[33]. Exploration involves finding new individuals so that uncharted areas in the search space are covered, whereas exploitation focuses on neighbouring points of previously visited areas. It is known that there is a good balance of these two strategies in evolutionary algorithms[31].

4. Results

Our experiments show that a hard X-ray FEL driven by an 8 GeV electron linac, is feasible by means of short-period in-vacuum undulators. 22 undulator cells (each 5 m long) with 1.1 m-long intersections are sufficient to achieve 1 Å wavelength. The findings are elaborated in the following.

Optimal SASE operation parameters (λ_u, g, P_{sat} and λ_{FEL}) are demonstrated in Figs 2-3 for vanadium permendur and iron, respectively. These results were obtained from 50 fittest solutions out of a population of 1k individuals as a result of 1k generations (total of 1M evaluations). In addition, it is clearly seen that plausible wavelength and saturation power values are feasible by short-period in-vacuum undulators. Figure 4 demonstrates that 1 Å wavelength is achievable along a saturation length of 110 m with 1.75 GW peak power.

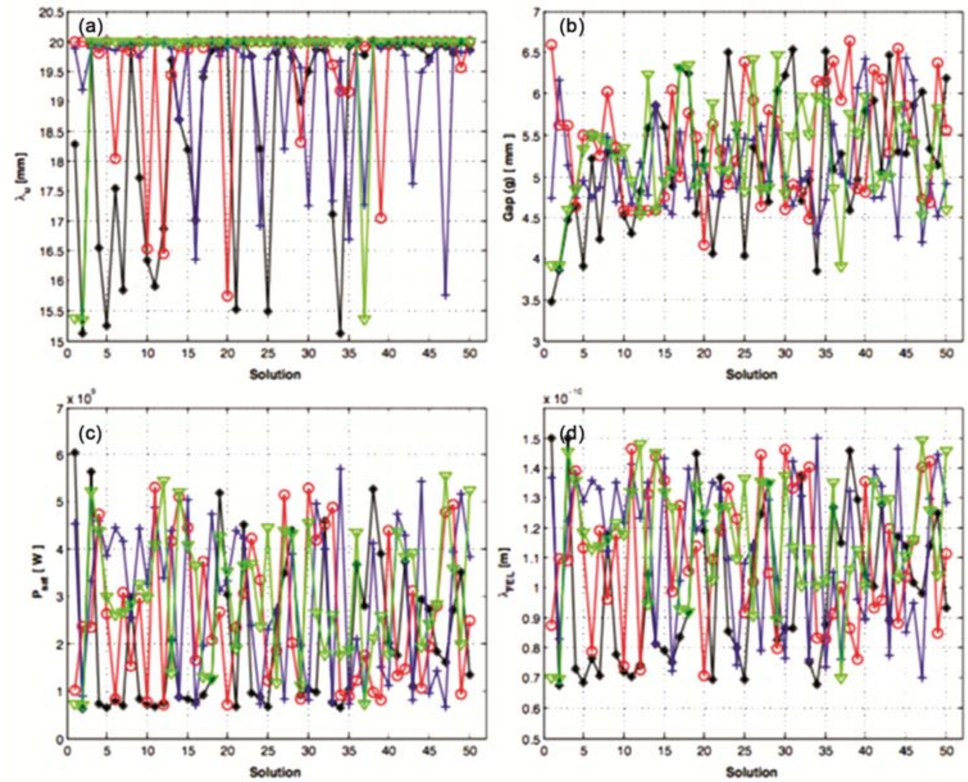

Fig. 3 — SASE performance parameters for hybrid with iron (*) NSGAII, (+) NSGAIII, (o) GDE3 and (∇) ε-MOEA. (a) λ_u (b) g (c) P_{sat} (d) λ_{FEL}

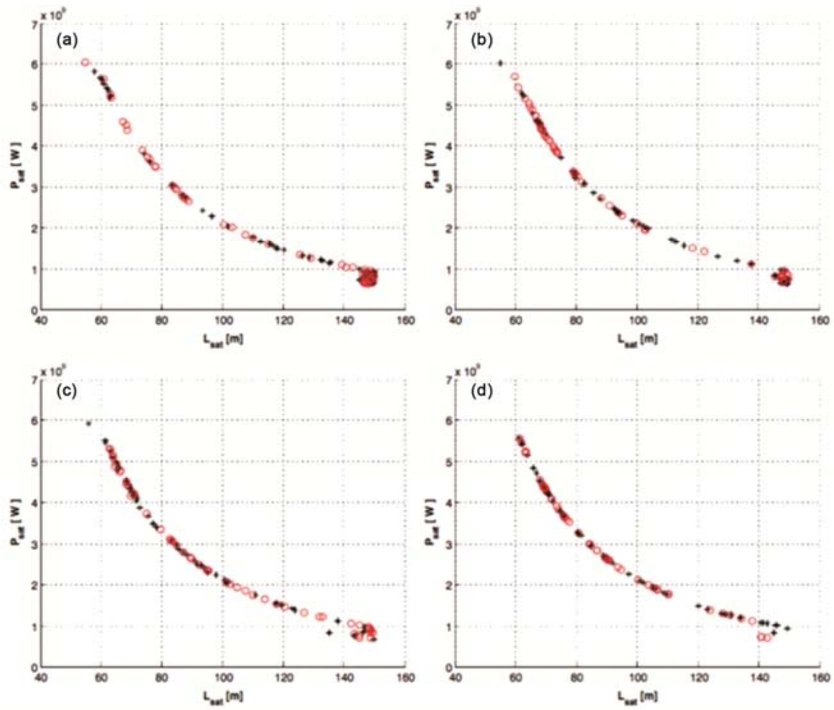

Fig. 4 — P_{sat} vs L_{sat} for hybrid with Vanadium Permendur (red circles) and hybrid with iron (black asteriks) undulators (a) NSGAII (b) NSGAIII (c) GDE3 (d) ε-MOEA. Note that each data point corresponds to an individual solution obtained by the evolutionary algorithm and should not be interpreted as a function of the axes.

5 Conclusions

Today, accelerator-based 4th generation light sources are quite in demand due to their superior radiation characteristics. Hence, a hard X-ray FEL generated by SASE operation is optimized using multiple objective evolutionary algorithms with an encoding scheme comprising of undulator period and gap for two different types of hybrid undulators.

Our findings reveal that short-period in-vacuum planar undulators achieve sub-Angstroms with plausible saturation power, Pierce parameter and saturation length using the optimized parameters. Conventional numerical approaches employ a fixed value for SASE parameters; however, the evolutionary approaches presented here use a range for these values and perform optimization in order to obtain Pareto optimal solutions for the given constraints on the ratio of gap and period as well as saturation power and length. Furthermore, it is found that the results obtained here are well-consistent with the operating X-ray FEL facilities around the world.

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