

OVERVIEW OF PERSEO, A SYSTEM FOR SIMULATING FEL DYNAMICS IN MATHCAD

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Abstract

Perseo is a library of functions devoted to the simulation of FEL dynamics in the *Mathcad* environment. Functions for the generation of phase space variables, for the solution of the pendulum-like equation and for manipulating the phase space in a number of devices are available. These function can be combined in order to model more complicated situations as time dependent simulations, 3D simulations, oscillator FEL configurations, optical klystron, cascaded FELs ...

INTRODUCTION

Mathematical computer aided scratchpads which integrate standard mathematical notation, text, graphs and programming capabilities in worksheets as *Mathcad* or *Mathematica* and *Matlab*, are widespread tools in the scientific community. Nowadays computers are fast enough to execute interactively from start-up to saturation an FEL simulation involving a few thousands macro-particles. This suggested to develop a set of basic functions which can be called from within the *Mathcad* environment, devoted to solve FEL dynamics related problems. The result is *Perseo*[1], a flexible tool that can be simply programmed to set up FEL simulations in a wide variety of configurations.

THE FEL MODEL IN PERSEO

The core of the library consists of a routine solving the pendulum-like FEL equations coupled with the field equations which govern the FEL longitudinal dynamics [2,3]. This routine includes self consistently the field variables for the higher order harmonics. In this picture the field is the superposition of slowly varying complex amplitudes $a_n = |a_n| e^{i\varphi_n}$ for each harmonic n , $E(z, t) = \sum_n \tilde{E}_n |a_n| e^{i(k_n z - \omega_n t + \varphi_n)}$. The parameters \tilde{E}_n link the dimensionless field amplitude a_n to the field at the harmonic n . They may be defined in terms of the saturation intensity [4] as $\tilde{E}_n = \sqrt{z_0 I_s(n) / 4\pi}$ where z_0 is the vacuum impedance. In a linear undulator the n^{th} harmonic saturation intensity is defined as $I_s(n) = 1 / (4\pi) (m_0 c^3 / r_0) (\gamma / N)^4 (\lambda_u K f_b(n, \xi))^{-2}$ where γ is the beam energy in $m_0 c^2$ units, λ_u is the undulator period, N is the number of undulator periods, K is the undulator parameter. The function $f_b(n, \xi) = J_{(n-1)/2}(\xi) - J_{(n+1)/2}(\xi)$ where $\xi = K^2 / 4(1 + K^2/2)$, is the Bessel factor arising from the average over the longitudinal fast motion typical

of linear undulators. The evolution of the amplitudes a_n is governed by the equations:

$$\begin{aligned} \frac{\partial \text{Re}(a_n(\tau))}{\partial \tau} &= -2\pi g_n \langle \cos(in\vartheta_i(\tau)) \rangle_i \\ \frac{\partial \text{Im}(a_n(\tau))}{\partial \tau} &= 2\pi g_n \langle \sin(in\vartheta_i(\tau)) \rangle_i \end{aligned} \quad (1)$$

where the variable $\tau = \beta_z c t / L_u$ is a dimensionless interaction time, $L_u = N\lambda_u$ is the undulator length and $c\beta_z$ is the longitudinal beam velocity. The phase $\vartheta_i = (k_L + k_u)z_i - \omega_L t$ is the electron phase in the ponderomotive bucket corresponding to the first harmonic field ($n=1$, $k_L = \omega_L/c = k_1 = 2\pi/\lambda_1$ is the wave-vector corresponding to the first harmonic and $k_u = 2\pi/\lambda_u$ is the wave-vector associated to the undulator period). The coupling coefficients at the odd harmonics g_n are given by [3]

$$g_n = 2\pi \left(\frac{N}{\gamma} \right)^3 [\lambda_u K f_b(n, \xi)]^2 \frac{I_{peak}}{I_A \Sigma_b} \quad (2)$$

where I_{peak}/Σ_b is the electron current density and I_A is the Alfvén current. The i^{th} particle motion is governed by pendulum-like equations:

$$\begin{aligned} \frac{d\vartheta_i}{d\tau} &= \nu_i \\ \frac{d\nu_i}{d\tau} &= \sum_n \cos(n\vartheta_i) \text{Re}(a_n) - \sin(n\vartheta_i) \text{Im}(a_n) \end{aligned} \quad (3)$$

where $\nu_i = 2\pi N (\omega_i - \omega_L) / \omega_i$ represents the frequency shift of the i^{th} particle resonance $\omega_i/c = 2\gamma_i^2 k_u / (1 + K^2/2)$ from the reference frequency ω_L . Note that the above choice for the coefficients (\tilde{E}_n, g_n) leads to the expression (3) for the particles dynamics, where all the harmonics in the expression of $d\nu_i/d\tau$ have the same weight factor. Analogous expressions for the helical undulator are easily obtained by substituting $f_b(n=1, \xi) = 1$, $K \rightarrow K_{helical} = \sqrt{2}K$ in (2) and in the definition of $I_s(n)$, and neglecting the higher order harmonic coupling ($f_b(n \neq 1, \xi) = 0$) in (2).

In the following we will analyze the subset of functions that are necessary for setting up a simple FEL simulation

in the *Mathcad* environment. Some knowledge of the basic *Mathcad* language is assumed [5].

The function FELPendulum_h

In *Perseo* the coupled equations (2) and (3) are solved by calling the function:

$$PHSP_{new} := FELPendulum_h(PHSP_{old}, g, \tau_0, \tau_1, tol) \quad (4)$$

This function integrates the coupled system of equations (2) and (3) with the coupling coefficients g (g is indeed an array with number of components equal to the number of simulated harmonics) advancing the system from τ_0 to τ_1 with tolerance tol . The variables $PHSP_{new}$ and $PHSP_{old}$ represent the status of the system before and after the integration and are defined as:

$$PHSP = \begin{pmatrix} n_h & \text{not used} \\ \text{Re}(a_1) & \text{Im}(a_1) \\ \vdots & \vdots \\ \text{Re}(a_{n_h}) & \text{Im}(a_{n_h}) \\ v_1 & \vartheta_1 \\ \vdots & \vdots \\ v_{n_p} & \vartheta_{n_p} \end{pmatrix} \quad (5)$$

The first line contains the number of harmonics n_h , then n_h lines contain the real and imaginary part of the field at each harmonic, followed by the coordinates (v, ϑ) of an arbitrary number of simulated particles n_p .

The function FELquietstart_h

The variable $PHSP$ may be prepared by filling the matrix with the desired field values and particles coordinates, but a more convenient way is that of using the function

$$PHSP := FELquietstart_h(v_0, \sigma_v, n_v, \vartheta_0, \vartheta_1, n_\vartheta, a) \quad (6)$$

that fills the variable $PHSP$ with $n_p = n_v \cdot n_\vartheta$ particles, n_v particles in the v space, over a Gaussian centred in v_0 with r.m.s. σ_v , and n_ϑ particles distributed uniformly in the interval $(\vartheta_0, \vartheta_1)$.

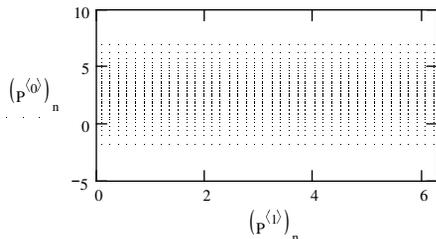


Figure 1: Phase space distribution obtained by calling the function *FELquietstart_h* with $v_0=2.6$, $\sigma_v=2$, $n_v=40$, $\vartheta_0=0$, $\vartheta_1=2\pi$, $n_\vartheta=40$.

A quiet start distribution is obtained by setting $\vartheta_1 = \vartheta_0 + 2n\pi$ with n integer (normally $\vartheta_0, \vartheta_1 = 0, 2\pi$).

An example of the phase space distribution as returned by *FELquietstart_h* is shown in Fig. 1.

A simple simulation

A simple simulation is realized by the *Mathcad* sequence in Fig. 2

```

v_0 := 2.6   sigma_v := 2   n_v := 40
n_theta := 40   theta_0 := 0   theta_1 := 2 * pi   a := ( 1 + 3i
                                                         0
                                                         0 )
P := FELquietstart_h(v_0, sigma_v, n_v, theta_0, theta_1, n_theta, a)
g_0 := ( 10
         0
         0 )
P := FELpendulum_h(P, g_0, 0, 1, TOL)
    
```

Figure 2: *Mathcad* sequence integrating the pendulum-like equation coupled to the field equations with coupling coefficient $g=10$ on the first harmonic and 0 on the higher harmonics.

The phase space in P is integrated over the undulator length with the coupling coefficient $g=10$ on the first harmonic and 0 on the higher harmonics. The resulting phase space is plotted in Fig. 3.

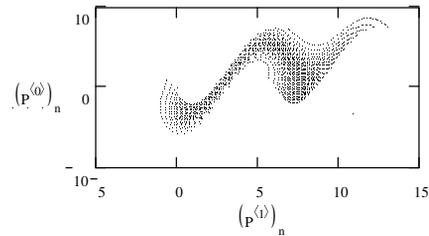


Figure 3: Phase space distribution at the end of the simulation with the parameters listed in Fig. 2.

After the FEL interaction the phase space is distributed in an interval longer than $(0, 2\pi)$. The periodicity in ϑ of the system of equations (2) and (3) can be imposed to the phase space variables with the function $P := FELBox_h(P, \vartheta_0, \vartheta_1)$. By calling this function with $(\vartheta_0, \vartheta_1) = (0, 2\pi)$ we obtain the phase space distribution of Fig. 4.

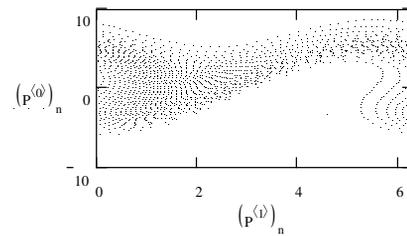


Figure 4: Phase space distribution after imposing a periodicity condition in the interval $(0, 2\pi)$.

Start-up from e-beam shot noise

Startup from shot noise may be simulated by using the function *FELquasiquietstart_h*($v_0, \sigma_v, n_v, \vartheta_0, \vartheta_1, n_\vartheta, \phi_{ns}, a$) which is analogous to the function *FELquietstart_h* except for the additional argument ϕ_n which is used to displace the particles according to the function

$$\vartheta_i = \arg(\phi_{ns}) + (1 - |\phi_{ns}|) \left[\left(\frac{\vartheta_1 - \vartheta_0}{n_\vartheta} \right) \left(i - \frac{n_\vartheta - 1}{2} \right) \right] \quad (7)$$

In the limit of small perturbation ($|\phi_{ns}| \rightarrow 0$) and sufficiently large number of particles n_ϑ the distribution has Fourier coefficients $b_n \equiv \phi_{ns}$ (bunching coefficients at the harmonic n) almost independent from n (see ref. [1]). The coefficient b_1 can be estimated in a steady state simulation using the procedure of ref.[6].

Inhomogeneous broadenings and three dimensional effects

The variable $v_i = 2\pi N(\omega_i - \omega_L)/\omega_i$ represents the relative shift of the resonance of the i^{th} particle from a given reference frequency ω_L . According to the definition of the resonant frequency of the i^{th} particle $\omega_i = 2\gamma_i^2 ck_u / (1 + K(x_i, y_i)^2/2 + \gamma_i^2(\theta_{x,i}^2 + \theta_{y,i}^2))$, where we have included the dependence on the angle between the average particle trajectory and the undulator axis $\theta_{xy,i} = \beta_{xy}/\beta_z$ (we use the notation $\theta_{xy,i} = \theta_{x,i}, \theta_{y,i}$) and the dependence of the undulator K parameter on the transverse coordinates, the particles distribution in energy and transverse phase space may be converted in a distribution in the detuning parameter space v . At the lowest order in x_i, y_i and $\theta_{xy,i}$ we have [7]

$$\begin{aligned} \sigma_{x,y} &= \sqrt{2\pi} N h_{x,y} \frac{2\gamma^2}{1+K^2/2} \left(\frac{\pi K}{\gamma \lambda_u} \right)^2 \left(\frac{\beta_{x,y} \varepsilon_{n,xy}}{\gamma} \right) \\ \sigma'_{x,y} &= \sqrt{2\pi} N \frac{2\gamma^2}{1+K^2/2} \left(\frac{\pi K}{\gamma \lambda_u} \right)^2 \left(\frac{\varepsilon_{n,xy}}{\beta_{x,y} \gamma} \right) \\ \sigma_e &= 4\pi N \frac{\sigma_\gamma}{\gamma} \end{aligned} \quad (8)$$

where $h_{x,y}$ are the undulator focusing parameters (with $h_x + h_y = 2$), $\varepsilon_{n,xy}$ and $\beta_{x,y}$ are the normalized emittances and the β Twiss coefficients in the x and y planes respectively. An approximated expression for standard deviation in the v space is obtained by combining quadratically the standard deviations (8)

$$\sigma_v \equiv \sqrt{\sigma_x^2 + \sigma_y^2 + \sigma_x'^2 + \sigma_y'^2 + \sigma_e^2} \quad (9)$$

In an oscillator FEL or in a seeded FEL and in general, when the transverse properties of the radiation may be considered as a constraint of the problem, the coupling coefficients (2) have to be corrected by a proper filling factor. In general when the radiation size is the result of the balance between diffraction and focusing induced by the gain, as in a single pass FEL, a filling factor coefficient may be derived from the Xie scaling laws [8] by calculating the ratio between the Xie factor with and without diffraction effects. In a similar way a coefficient correcting the coupling factor g may be derived from the semi-analytical model in [9].

TIME DEPENDENT SIMULATIONS

Mathcad programming may be used to set up FEL simulations in a wide variety of conditions. As an example we analyse the case of 1D FEL simulations including pulse propagation effects. The field is governed by the evolution equation

$$\left(\frac{\partial}{\partial \tau} + \Delta \frac{\partial}{\partial \zeta} \right) a_n(\tau, \zeta) = -2\pi g_n I(\zeta) \langle \exp(in\vartheta_i(\tau, \zeta)) \rangle_\zeta \quad (10)$$

where $\Delta = N\lambda_i$ is the slippage length, ζ is the longitudinal coordinate in the frame moving with the electron bunch and $I(\zeta)$ is the normalized current shape. The average on the r.h.s. of (10) is intended in a region λ_i at the position ζ . The solution of this equation is obtained by defining an array of variables of the type of *PHSP* in (5), representing the sampling of both the field and the beam phase space variables along the coordinate ζ at the positions $\boldsymbol{\zeta} = \zeta_0, \zeta_1, \dots, \zeta_{nb-1}$. The phase space beamlets are defined as

$$\mathbf{P} = (P_0, P_1, \dots, P_{nb-1}) \quad (11)$$

The undulator is divided in time steps such that the step length $\Delta\tau$ is related to the spatial sampling $\Delta\zeta$ by the condition $\Delta\zeta = \Delta/\Delta\tau$. With such a choice, at each time step the field variables at the i^{th} position in the \mathbf{P} array have to slip to the next position: $i^{\text{th}} \Rightarrow i^{\text{th}}+1$. For this purpose the function in Fig. 5 is defined.

$$\boxed{\begin{array}{l} \text{FELSlipField}(P1, P2) := \text{for } n \in 1..P1_{0,0} \\ \left| \begin{array}{l} P1_{n,0} \leftarrow P2_{n,0} \\ P1_{n,1} \leftarrow P2_{n,1} \end{array} \right. \\ P1 \end{array}}$$

Figure 5: Function *FELSlipField* loading the field data from beamlet $P2$ to $P1$. Fields in $P2$ are overwritten.

The simulation of a single pass FEL in time dependent mode is then simply obtained with the function shown in Fig. 6. The first loop over the nb beamlets loads the initial phase space array \mathbf{P} , generating each beamlet with a

different shot noise coefficient $\phi_{n,i}$. The initial field amplitude a_0 is multiplied by a modulating coefficient se_i which can be defined in order to simulate the ζ dependence of an input seed. The second loop over the variable n_τ takes care of the integration of the phase space beamlets P along the undulator. At each time step of length $\Delta\tau$ the array of beamlets P is stored in the matrix **OUT**, particles and fields are advanced by the *FELpendulum_h* and the slippage is applied by the *FELSlipField* procedure defined in Fig. 5. Each column of the matrix **OUT** contains the array P at time $\Delta\tau n_\tau$. As an example of a simulation obtained with the routine in Fig. 6, we have considered the case of a SASE FEL with the resonance at 200 nm, a FEL parameter $\rho \approx 4 \times 10^{-3}$ and gain length of about 0.3 m. In Fig. 7 the longitudinal phase space at saturation is shown. The beamlets at the same time frame have been joined together in the same plot. The horizontal axis represents the beamlets position along ζ . The phase space variable ϑ in each beamlet is expanded by the factor $\Delta\zeta/2\pi$ in order to give the impression of a continuous beam. The ζ window is large

enough to contain two spikes, the red line represents indeed the separatrix of the motion and is proportional to the root of the field.

```

FELTimeDep :=
  for i ∈ 0..nb - 1
    Pi ← FELquasiquietstart_h (v0, σv, nv, 0.0, 2·π, nθ, φn,i, a0·sei)
  τ ← 0
  for nτ ∈ 0..nT
    for i ∈ 0..nb - 1
      OUTnτ,i ← Pi
      Pi ← FELpendulum_h (Pi, g1, τ, τ + Δτ, TOL)
    for n ∈ nb - 1..0
      PT ← FELSlipField (Pi, Pif(i≠0, nb-1, i-1))
      Pi ← FELbox_h (PT, 0, 2·π)
    τ ← τ + Δτ
  OUT

```

Figure 6: Function simulating the longitudinal dynamics of a single pass FEL in time dependent mode. The result returned by the matrix **OUT** contains the beamlets phase spaces composing the beam at the n_T time steps.

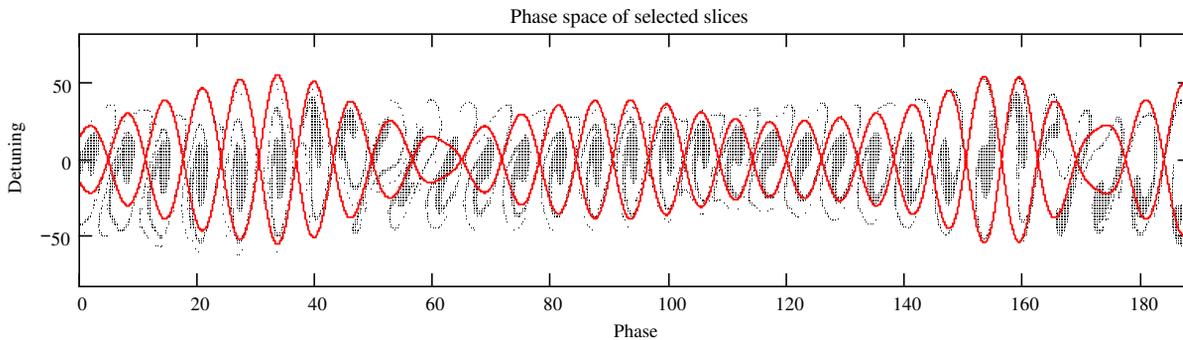


Figure 7: The beamlets resulting after a SASEFEL simulation at saturation have been joined together in the same plot. The horizontal axis represents the beamlets position along ζ . The phase space variable ϑ in each beamlet is expanded by the factor $\Delta\zeta/2\pi$ in order to give the impression of a continuous beam. The red line represent the separatrix of the motion and is proportional to the root of the field.

CONCLUSIONS

We have provided a brief overview of the physical model implemented in *Perseo*. The main functions required for setting up a simple simulation have been analysed and the algorithm for implementing time dependent simulation has been explained. With a similar procedure fully 3D simulations can be implemented but the cpu and memory requirements becomes excessive for an interactive execution.

For additional information and further insight in *Perseo* capabilities the reader is addressed to the web page [1] and to the *Perseo* Electronic Handbook included in the installation package.

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