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Description of FEL3D
A Three Dimensional Simulation Code for TOK and FEL

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1. Introduction

FEL3D is a three dimensional simulation code, written for the purpose of calculating the parameters of coherent radiation emitted by electrons in an undulator.

The program was written predominantly for simulating the coherent super-radiant harmonic frequency emission of electrons which are being bunched by an external laser beam while propagating in an undulator magnet. This super-radiant emission is to be studied in the TOK (transverse optical klystron) experiment, which is under construction in the NSLS department at Brookhaven National Laboratory. The program can also calculate the stimulated emission radiometric properties of a free electron laser (FEL) taking into account three dimensional effects. While this application is presently limited to the small gain operation regime of FEL's, extension to the high gain regime is expected to be relatively easy.

The code is based on a semi-analytical concept. Instead of a full numerical solution of the Maxwell-Lorentz equations, the trajectories of the electron in the wiggler field are calculated analytically, and the radiation fields are expanded in terms of free space eigenmodes (Hermite-Gaussian modes, or plane waves). This approach permits efficient computation, with a computation time of about 0.1 sec/electron on the BNL IBM 3090.

The code reflects the important three dimensional features of the electron beam, the modulating laser beam, and the emitted radiation field (see discussion in Chapter 3). The statistical approach is based on averaging over the electron initial conditions according to a given distribution function in phase space, rather than via Monte-Carlo simulation. The present version of the program is written for a uniform periodic wiggler field, but extension to nonuniform fields (transverse gradient, tapering, random errors) is straightforward.

2. The Physical Problem

In this chapter we summarize the theoretical modeling and concepts underlying the computer program. A more detailed description of the theory can be found in earlier publications [1,2].

2.1 Undulator, Super-radiant and Stimulated (FEL) Radiation

We define here the physical structure and the radiation schemes to which the present discussion is relevant. Fig. 1 describes two different embodiments of the TOK, the device on which most of the attention was focused in the present stage of code development. The main part of the optical klystron is the undulator (wiggler) magnet, which induces transverse quiver motion in the electron trajectories.

The transverse quiver motion of a single electron produces coherent Doppler shifted radiation emitted predominantly in the forward direction (undulator synchrotron radiation). This radiation is emitted at a central frequency

$$\omega_u = \frac{k_w c}{\beta_z^{-1} - 1} \approx 2\gamma_z^2 k_w c \quad (1)$$

oscillating at the undulator harmonic frequency and its odd harmonics $\omega_{ul} = l\omega_u$. Here $k_w \equiv 2\pi/\lambda_w$ is the wiggler wave number, $\beta_z \equiv v_z/c$, $\gamma_z = (1 - \beta_z^2)^{-1/2}$, and l is an odd integer.

While the undulator synchrotron radiation emitted from a single electron is temporarily and spatially coherent, different electrons, entering the wiggler at random times, emit at random phase relative to each other. Consequently the undulator radiation from an electron beam is only partially coherent. The emission from the electron beam can be made coherent if the electrons are bunched in space (in the axial dimension) and time. When this happens the radiative emission from the different electrons can interfere constructively in the forward direction, producing "super-radiant emission". In the optical klystron the bunching of the electrons is done by means of an external laser oscillating at approximately one of

1 (a)

1 (b)

Fig. 1. Schemes for super-radiant (bunched beam) coherent harmonic generation.

the undulator harmonic frequencies $\omega_m \equiv m\omega_u$. The laser beam is focused at the first undulator section (in the scheme of Fig. 1a), or near the undulator entrance (in the scheme of Fig. 1b). The combined force of the wiggler and laser beam fields (ponderomotive force) modulates the energy of the electrons at the laser frequency. This energy modulation becomes density modulation in the second undulator section (Fig. 1a) or towards the end of the undulator (Fig. 1b). If the density modulation is tight enough, it contains harmonics of the laser frequency. Consequently, the bunched electrons emit super-radiant coherent radiation at the laser frequency ω_m , and its odd harmonics $n\omega_m$. The definitions of the different harmonics involved in undulator-synchrotron radiation and super-radiant emission are summarized in Table 1.

Table 1: Frequencies Involved

Frequency	Notation/Definition	Linewidth
Fundamental undulator frequency	$\omega_u = \frac{k_w c}{\beta_z^{-1} - 1} \approx 2\gamma_z^2 k_w c$	$\frac{\Delta\omega_u}{\omega_u} = \frac{1}{N_w}$
Modulating laser frequency	$\omega_m \approx m\omega_u$	$\frac{\Delta\omega_m}{\omega_m} = \frac{2\pi/T_{laser}}{\omega_n}$
n-th order coherent harmonic of modulator	$\omega_n = n\omega_m (\approx nm\omega_u)$	$\frac{\Delta\omega_n}{\omega_n} = \frac{2\pi/T_{pulse}}{\omega_n}$
l-th order incoherent harmonic of wiggler	$\omega_{ul} = l\omega_u$	$\frac{\Delta\omega_{ul}}{\omega_{ul}} = \frac{1}{lN_w}$

The FEL may be viewed as an elaboration of the optical klystron. The optical beam of an external laser (oscillating again at $\omega_m \approx m\omega_u$) bunches the electron beam in the same way as it does in the TOK. However, we are concerned only with coherent radiation, which is emitted at the same frequency and into the same spatial-angular domain of the modulating radiation beam. This radiation adds up in phase with the input optical field and results in "amplifier gain" (in the present version of the program the added radiation power is

assumed small relative to the input power and does not affect the bunching). The different radiative emission schemes of an electron beam (spontaneous, super-radiant, stimulated) are summarized in Table 2.

Table 2: Classical Definitions of Radiation Schemes

(1) **UNDULATOR SYNCHROTRON RADIATION**

(FEL SPONTANEOUS EMISSION): The temporally incoherent radiation of electrons entering into a wiggler/undulator at random.

(2) **SUPER-RADIANT FREE ELECTRON RADIATION:** The temporally coherent radiation of bunched electrons oscillating in phase with each other in a wiggler/undulator.

(3) **FREE ELECTRON LASING:** The coherent emission of bunched electrons radiating in phase into the same frequency and spatial domain as the radiation field which produced the bunching.

2.2 The Electron Trajectories and Equations of Motion

The electron transverse trajectories are assumed to be unaffected by the interaction with the radiation field. Typically, this is the trajectory of an electron undulating and freely propagating in a wiggler. The transverse coordinates of the electron $x_j(t) = \bar{x}_j(t) + x_{wj}(t)$, $y_j(t) = \bar{y}_j(t) + y_{wj}(t)$, is composed in general of an averaged (over undulator period) motion $(\bar{x}_j, \bar{y}_j)$ and undulator motion (x_{wj}, y_{wj}) .

In its present version the program is written for a uniform planar wiggler. For this case the transverse trajectories can be described by analytic expressions:

$$\bar{x}_j = x_{j0} + c\beta_{j0}\phi_{x_{j0}}(t - t_{j0})$$

$$x_{wj} = -\frac{a_w}{\gamma k_w} \sin(k_w z_j(t))$$

$$\bar{y}_j = y_{j0} + c\beta_{j0}\phi_{y_{j0}}(t - t_{j0})$$

$$\beta_{wj} = \frac{a_w}{\gamma} \cos(k_w z_j(t))$$

$$y_{wj} = 0 \quad (2)$$

The modulating laser beam field is taken to be a general fundamental Hermite-Gaussian mode with independent x and y focusing parameters:

$$E_m(x, y, z, t) = \hat{e}_x E_0 \frac{w_{xm}(0)w_{ym}(0)}{w_{xm}(z)w_{ym}(z)} \times \\ \times \operatorname{Re} \left[\exp \left\{ -\frac{x^2}{w_{xm}^2(z)} - \frac{y^2}{w_{ym}^2(z)} + i\Phi(x, y, z) + i\frac{\omega_m}{c}z - i\omega_m t \right\} \right]$$

$$\Phi(x, y, z, \omega_m) = \frac{1}{4} \frac{\omega_m}{c} \left(\frac{x^2}{R_x(z)} + \frac{y^2}{R_y(z)} \right) - \frac{1}{2} \left[\arctan \left(\frac{z - z_{w_x}}{z_{R_x}} \right) \right. \\ \left. + \arctan \left(\frac{z - z_{w_y}}{z_{R_y}} \right) \right]$$

$$R_{x,y} = (z - z_{w_{x,y}}) \left(1 + \frac{z_{R_{x,y}}^2}{(z - z_{w_{x,y}})^2} \right)$$

$$[z_R(w_m)]_{x,y} = \pi \frac{[w_{0m}]_{x,y}^2}{\lambda_m} \quad (3)$$

Since the wiggler field and the radiation field of the modulating laser beam are both transverse, the only time averaged (over optical frequencies) force that the radiation and

wiggler fields can apply on the electron is the longitudinal cross term of the two fields. Consequently, the optical modulation problem requires solution only of the axial coordinate trajectories $z_j(t)$. These trajectories are obtained by solving the energy equation and the longitudinal component of the Lorentz equation with the radiation field (3) and the transverse coordinates specified by (2).

The main effect of longitudinal optical modulation and bunching may be attributed to the second order "beat force" or "ponderomotive force" applied on the electrons by the combined Lorentz force effect of the wiggler and radiation field. This force wave can be synchronous with the electrons and thus, subjects them to a pendulum equation motion in the z dimension. For an intense planar wiggler with

$$\bar{a}_w = \frac{e\bar{B}_w}{k_w m_e} > 1 \quad (4)$$

an additional feature complicates the simple pendulum equation picture. This is the effect of longitudinal quiver of the electron in the wiggler with frequency $2k_w v_z$. This quiver makes it possible to apply effective longitudinal pendulum forces not only at the fundamental frequency ω_u but also at its odd harmonics. However, the electron force equation now includes many pendulum forces and its solution becomes more difficult.

Two formulations were developed for the solution of the axial electron trajectories (modulation and bunching): (1) an exact set of equation, describing the electron trajectories under the combined effect of all the longitudinal force terms, which arise due to the longitudinal quiver; (2) an averaged set of equations, describing the electron trajectories under the effect of a single pendulum effective force at one of the harmonic frequencies. The amplitude of the effective force was obtained by analytical averaging over the longitudinal quiver period.

The two sets of equations for the longitudinal trajectories (bunching) calculation are:

(1) Exact equations

$$\begin{aligned}
\frac{d\gamma_j}{d\tau} &= -\frac{e}{m_e} a_w E_m(r_{\perp j}(t)) [\cos(\psi_{+j} + \phi(r_{\perp j}(t))) - \cos(\psi_{-j} + \phi(r_{\perp j}(t)))] \\
\frac{du_{zj}}{d\tau} &= -\frac{e}{m_e} a_w E_m(r_{\perp j}(t)) \left[\left(1 + \frac{k_w c}{\omega_m}\right) \cos(\psi_{+j} + \phi(r_{\perp j}(t))) - \left(1 - \frac{k_w c}{\omega_m}\right) \cos(\psi_{-j} - \phi(r_{\perp j}(t))) \right] \\
&\quad - \frac{1}{2} a_w^2 k_w c \sin(\psi_{+j} - \psi_{-j}) \\
\frac{d\psi_{+j}}{d\tau} &= c \left(\frac{\omega}{c} + k_w \right) u_{zj} - \omega_m \gamma_j \\
\frac{d\psi_{-j}}{d\tau} &= c \left(\frac{\omega}{c} - k_w \right) u_{zj} - \omega_m \gamma_j
\end{aligned} \tag{5}$$

The phases $\psi_{\pm}$ are defined by $\psi_{\pm j} \equiv (\omega/c \pm k_w)z_j - \omega t$, and $u_{zj} = p_{zj}/m_e = \gamma_j \beta_{zj}$. Consequently the position and time can be found from the solution of (5) by using

$$\begin{aligned}
z_j &= \frac{\psi_{+j} - \psi_{-j}}{2k_w} \\
ct_j &= \frac{(1 - k_w c/\omega_m) \psi_{+j} - (1 + k_w c/\omega_m) \psi_{-j}}{2k_w}
\end{aligned} \tag{6}$$

The independent variable in this set of equations is the relativistic proper time $\tau = \int_{t_{0j}}^t dt' / \gamma_j(t') \approx \int_0^z dz' / cu_j$. The integration of Eq. 5 for each electron should be carried out until $z_j(\tau) = L$ (the end of the wiggler).

(2) Averaged equations

When analytical averaging of the longitudinal quiver is carried out, an approximate set of equations with a single pendulum driving force is obtained:

$$\left\{ \begin{aligned} \frac{d\gamma_j}{d\tau} &= \frac{1}{2} (-1)^{\frac{n-1}{2}} \frac{E_m(x_j(t), y_j(t))}{m_e} a_w \left[\frac{J_{n-1}(u)}{2} - \frac{J_{n+1}(u)}{2} \right] \sin [\psi_{mj} + \Phi_{mj}(x_j, y_j, z_j, \omega_m)] \\ \frac{d\psi_{mj}}{d\tau} &= \frac{k_m + mk_w}{m_e} p_z - \omega_m \gamma \\ \left[\frac{J_{n-1}(u)}{2} - \frac{J_{n+1}(u)}{2} \right] \omega_m p_z - \left[(k_m + k_w) \frac{J_{n-1}(u)}{2} \right. \\ &\quad \left. - (k_m - k_w) \frac{J_{n+1}(u)}{2} \right] m_e^2 \gamma = \text{const}_j \end{aligned} \right.$$

$$\psi_{mj} \approx (k_m + mk_w) z_j(t) - \omega_m t$$

$$\tau \equiv \int_{t_{j0}}^t \frac{dt'}{\gamma_j(\theta')} = \text{proper time}$$

$$u \equiv \frac{\omega_m}{8k_w} \frac{a_w^2}{c\beta_z \gamma^2} \approx \frac{m}{4} \frac{a_w^2}{1 + a_w^2/2} \quad (7)$$

This set of equations needs to be solved with the initial conditions: $\psi_{mj}(\tau = 0) = \psi_{mj0} = -\omega_m t_{j0}$; $\gamma_j(\tau = 0) = \gamma_{j0}$; $z_j(\tau = 0) = 0$. It is basically a standard pendulum equation with slowly varying amplitude and phase, both of which depend on the electron transverse trajectories. The fast longitudinal quiver, which is the essential source of the odd harmonic undulator radiation emission when $K \ll 1$, was averaged away in the derivation of Eq. 7

(off the force equations), leaving the various Bessel function factors, and producing the average constant of the motion of Eq. (7) [8].

While the first set of equations provide accurate prediction of the electron modulation and bunching parameters, it necessarily requires a lengthy computational process: integration steps must be small relative to the longitudinal quiver period. The second set of equations provides less accurate predictions, but assures faster computation. In the present stage of development only the program written on the basis of the second set of equations has been coded, debugged, and operated with all 3-D features.

2.3 Statistical Averaging

The statistical averaging approach taken in FEL3D is based on numerical averaging of all computed parameters over all the initial conditions of the sample electrons weighed by the given distribution function of the electron beam at the entrance to the wiggler. This approach should result in the predicted values of the parameters to be measured in the experiment. If, in the experiment, the measured parameter value fluctuates because of fluctuations in the e-beam distribution function, the computed parameters should correspond to the measured parameters averaged over many experiments.

The distribution function averaging adopted here is more appropriate than the Monte Carlo approach, which is sometimes taken in simulation programs. In the Monte Carlo approach, one distributes electron initial conditions via a random number generator weighed by the known statistical distribution function. This introduces an amount of noise in the computed values of physical parameters. Since, however, the noise in the measured parameters is determined by the fluctuations in the actual electron beam (shot noise), and since these fluctuations are much smaller than those induced by the Monte Carlo method, our approach should produce a closer match between computed and measured values of physical parameters.

To obtain proper sampling of the distribution function, enough sample electrons must be taken. It is assumed that the electrons are injected into the wiggler entrance with a uniform distribution in the time (or initial phase $\psi_{j0} = \omega_m t_{j0}$) domain (no prebunching of the beam). For a given choice N_ϕ of electrons representing the initial phase distribution in one optical period, a one period phase region $-\pi/2 < \psi_{j0} < 3\pi/2$ is divided into N_ϕ equal segments, and one electron is placed in the center of each segment. This procedure assures avoiding unintended prebunching of the sample electron beam. The number of electrons N_ϕ to be chosen depends on the highest harmonic-frequency bunching and emission to be calculated, and the accuracy required of the computation. The Nyquist theorem suggests that a minimum (and usually sufficient) number of sampling electrons is

$$N_\phi = 4n \quad (8)$$

where n is the highest laser harmonic number which is of relevance in the bunching and radiative emission process.

Arbitrary distribution functions can be used for sampling the electron initial conditions in the transverse coordinates (x_{0j}, y_{0j}) , angles (ϕ_{x0j}, ϕ_{y0j}) , and energy γ_{0j} . The present program is written with an assumption of Gaussian distribution in all five variables. This is a good approximation, especially for storage ring beams.

For proper sampling of the Gaussian distribution function the normalized Gaussian $F(z) = e^{-z^2}/\sqrt{\pi}$ is divided into N equal area segments (see Fig. 2), where N is the number of electrons being sampled in a given dimension $(x, y, \phi_x, \phi_y, \gamma)$. One sample electron is then placed in the center of gravity of each of the N equal area segments.

There is no simple estimate on the number of electrons required for representative sampling in each phase space dimension. A choice of 8 electrons per dimension gave

Fig. 2. Sampling algorithm in GAUSS: The distribution is split into $N=8$ equal area sections and the sampling electrons are located in the center of gravity of each section.

consistent results for same computations of on-axis radiative emission. More sampling points may be required for a reliable estimate of off-axis radiation parameters.

Since the wiggler structure, the modulating laser beam, and the distribution functions all satisfy symmetry of reflection $x \rightarrow -x$ and $y \rightarrow -y$, the dynamics of an electron with initial condition (x_0, ϕ_{x0}) is identical to that of an electron at $(-x_0, -\phi_{x0})$. Consequently, the simulation code can take advantage of this symmetry and sample only half of the phase space distribution in both (x, ϕ_x) and (y, ϕ_y) planes (see Fig. 3).

The 5-D electron distribution function in the wiggler factorizes at any plane z as

$$f_x(x, \phi_x) f_y(y, \phi_y) f_\gamma(\gamma) \quad (9)$$

The distribution functions of each of the conjugate phase space variables $f_x(x, \phi_x) f_y(y, \phi_y)$ factorize at a waist point z_{0x}, z_{0y} , which may in general be different if the focusing parameters of the beam are different in the two transverse dimensions. This is usually the case with storage ring beams. While the sampling procedure described above is carried out for each phase space dimension at its corresponding waist position (z_{0x} or z_{0y}), the initial conditions at $z = 0$, which are to be used for the simulation code, are computed by the back tracing transformation

$$\begin{aligned} x_j(0) &= x_{j0} - z_{w_x} \phi_{x_{j0}} \\ \phi_{x_j}(0) &= \phi_{x_{j0}} \end{aligned} \quad (10)$$

where $(x_{j0}, \phi_{x_{j0}})$ are the coordinates at the waist and $(x_j(0), \phi_{x_j}(0))$ are the coordinates at $z = 0$. Corresponding expressions apply in the y dimension with the substitution $x \rightarrow y$. The effect of linear free propagation (Eq. 10) on the beam distribution in phase space is illustrated in Fig. 4.

Fig. 3. The meaning of symmetry in initial conditions: when symmetry ($x \rightarrow -x$, $x' \rightarrow -x'$) is taken advantage of, only the shaded part of the distribution is sampled, representing the entire distribution.

2.4 The Radiation Parameters

A general formulation for calculating the radiation parameters of the coherent (super-radiant) and incoherent (spontaneous) harmonic emission of a wiggler is described in ref. [4]. The formulation enables calculation of radiation into arbitrary direction (plane waves) or, alternatively, an arbitrary set of orthogonal modes (Hermite-Gaussian). The radiation parameters that can be calculated are the total power (P), radiant intensity ($dP/d\Omega$), brightness ($d^2P/dAd\Omega$), and their corresponding spectral counterpart parameters ($d/d\omega$).

The following is a list of the parameters, which can be computed from the data produced by the simulation program, along with the formulas used for the computation, and an explanation of the parameters used. Parameters marked with an asterisk have not yet been coded into the program.

(1) The bunching parameter for on-axis emission

$$\eta_n(z) \equiv \frac{\tilde{I}_{zn}(z)}{I_0(z)} = 2 \left\langle e^{-in\psi_m} \right\rangle \quad (11)$$

This parameter gives the Fourier component of the longitudinal current at the n -th harmonic frequency of the modulating laser beam ($\omega_n = n\omega_m$). The wave number of the bunched current, the amplitude of which is calculated, is $\omega_n/c - k_w$, corresponding to a current source which when wiggled by a wiggler of wave number k_w , emits plane wave radiation in the forward direction ($\underline{k} = \hat{e}_z \omega_n/c$, $\omega = \omega_n = n\omega_m$).

The averaging is done by computing

$$\langle () \rangle_i = \frac{1}{N} \sum_{i=1}^N ()$$

where $j = 1, \dots, N$, are the sampling electrons determined as described in Section 2.3.

(2) The radiation parameter for on-axis emission

$$r_n(z) \equiv \frac{1}{\lambda_w} \int_0^z \eta_n(z') dz' \quad (12)$$

This parameter measures the amplitude of constructive interference of radiation emitted by the electrons as they propagate along the wiggler. In measuring the constructive interference amplitude, the reference is to radiative emission of plane waves in the forward direction. Note that in order to maximize the radiation parameter modulus $|r_n(z)|$, it is not sufficient to maximize the bunching parameter amplitude $|\eta_n(z)|$, but its phase must also be kept constant along a substantial section of the wiggler.

(3) The radiant intensity on-axis

$$\left(\frac{dP_{S.R.}}{d\Omega} \right)_{\Theta=0} = \frac{1}{16} \sqrt{\frac{\mu_0}{\epsilon_0}} \left(n \frac{\lambda_w}{\lambda_m} \right)^2 I_0^2 \left(\frac{\bar{a}_w}{\gamma \beta_z} \right)^2 [JJ]_l^2 |r_n(z)|^2 \quad (13)$$

Here $[JJ]_l \equiv J_{l-1/2}(lu) - J_{l+1/2}(lu)$ where $l \equiv mn$ is the undulator harmonic number and $\sqrt{\mu_0/\epsilon_0}$ is the vacuum impedance. Note that the super-radiant emission is proportional to the square of the instantaneous current of the e-beam - I_0^2 .

*(4) Spectral radiant intensity

$$\left(\frac{d^2 P_{S.R.}}{d\Omega d\omega} \right) = \frac{1}{2\pi} \sigma_t \left(\frac{dP_{S.R.}}{d\Omega} \right) \quad (14)$$

The coherence time of the super-radiant emission is σ_t , where σ_t is the standard deviation of the electron pulse. This is so assuming $l_{coh,L} \gg cl_t \gg N_w \lambda_n$ where $l_{coh,L}$ is the coherence length of the modulating laser. The corresponding bandwidth is $\Delta\omega = 2\pi/\sigma_t$.

(5) Radiant intensity of spontaneous undulator radiation on-axis

$$\left(\frac{dP_{U.R.}}{d\Omega}\right)_{\Theta=0} = \frac{1}{4} \sqrt{\frac{\mu_0}{\epsilon_0}} \frac{c \lambda_w^2}{\lambda_l^3} e I_0 \left(\frac{a_w}{\gamma}\right)^2 [JJ]_l^2 N_w \quad (15)$$

This parameter is calculated for the purpose of comparison to the super-radiant emission parameters.

(6) Ratio of super-radiant to spontaneous emission

$$\frac{\left(\frac{dP_{S.R.}}{d\Omega}\right)_{\Theta=0}}{\left(\frac{dP_{U.R.}}{d\Omega}\right)_{\Theta=0}} = \frac{1}{4} \frac{I_0 \lambda_w}{ec} \frac{1}{N_w} |r_n(L)|^2 \quad (16)$$

This parameter gives the ratio by which a detector reading will be increased when the modulating laser is turned on, and the detector is placed on the wiggler axis in the far field.

If the radiation is measured through a filter or spectrometer of bandwidth $\Delta\omega_{\text{filter}} < \omega_m/N_w$, (ω_m/N_w is the bandwidth of the spontaneous undulator radiation), then the measured enhancement ratio (16) will be increased by a factor $\frac{\omega_m}{N_w \Delta\omega_{\text{filter}}}$

*(7) Average energy loss of the e-beam

$$\langle\Delta\gamma\rangle = \langle\gamma_i(z) - \gamma_i(0)\rangle \quad (17)$$

The total induced power emission by the beam (in all directions at the modulating frequency) is computed from

$$\Delta P_{\text{tot}} = \frac{m_e^2}{e} \langle\Delta\gamma(L)\rangle I_0 = 0.511 \langle\Delta\gamma(L)\rangle I_0 \times 10^{-6} \quad (18)$$

*(8) Standard deviation of energy spread after interaction

$$\sigma_\gamma(L) = \left\langle (\gamma_i(L) - \bar{\gamma}(L))^2 \right\rangle^{1/2} \quad (19)$$

This parameter may be useful for estimating the effect of the modulating laser beam on anomalous bunch broadening and storage ring operation.

(9) The bunching parameter for a given transverse mode $\bar{E}_{q_R}(\underline{r}, \omega_n)$

$$\eta_{qn_R}(z) = 2 \left\langle \epsilon_{q_R}(x_j, y_j, z, \omega_n) e^{-i(n\psi_{m_j} + \phi_j)} \right\rangle_j \quad (20)$$

Here ϵ_{q_R} is the dimensionless profile function of a free space transverse radiation mode q : $\bar{E}_{q_R} = E_0 \epsilon_{q_R} e^{ikz + i\phi}$, where $\bar{E}_q(\underline{r})$ is one of a set of orthogonal transverse modes by which we choose to expand the radiation field (e.g. Hermite-Gaussian modes). The modes are assumed to be polarized in the electron wiggling plane, and their waist size and waist position may be arbitrarily chosen to match the radiation field (in order to require as few modes as possible for the expansion of the radiation field). The mode waist size and position may be (and usually is) different from the waist size and position of the modulating laser beam and therefore are distinguished by the subscript R. Arbitrary normalization may be chosen for the modes. In the subsequent equations we define an effective mode area by

$$\iint |\epsilon_q(x, y)|^2 dx dy = A_{em} \quad (21)$$

This mode area depends in general on the mode normalization and is therefore a function of the mode number. In the present application we use (21) as a means for mode normalization, and particularly for Hermite-Gaussian modes we choose to define for all modes

$$A_{em} = \frac{\pi}{2} w_{0x_R} w_{0y_R} \quad (22)$$

This normalization corresponds to a normalization of the fundamental Gaussian to maximum field at the waist center of E_0 [V/m] and mode power $p = 1/2 \sqrt{\epsilon_0 \mu_0} A_{em} E_0^2$ [watts].

The radiation parameter η_{qn} gives the temporal Fourier component of the longitudinal current at the n -th harmonic frequency of the modulating laser beam ($\omega_n = n\omega_m$). The spatial phase and amplitude of this component are matched to excite the q_R order transverse radiation mode.

(10) The radiation parameter for a given transverse mode.

Similarly to (12)

$$r_{qn_R}(z) = \frac{1}{\lambda_w} \int_0^z \eta_{qn_R}(z') dz' \quad (23)$$

This parameter measures the amplitude of constructive interference of radiation emitted coherently into transverse mode q by electrons propagating along the wiggler.

*(11) The super-radiant power emission into a transverse radiation mode

$$(P_{S.R.}(z))_{qn} = \frac{1}{\gamma} \sqrt{\frac{\mu_0}{\epsilon_0}} \lambda_w^2 \left(\frac{a_w}{\gamma_0 \beta_{z0}} \right)^2 I_0^2 [JJ]_I^2 |r_{qn}(z)|^2 \quad (24)$$

This parameter is useful if the particular mode q can be isolated experimentally by spatial filtering techniques and measured or utilized, or alternatively, if the character of the radiation field, and the choice of the waist size and position are such that predominantly a single radiation mode (e.g. the fundamental Gaussian mode) is excited.

The advantage of the mode expansion characterization is that all the optical properties of the radiation field are well defined if the single mode description is a good approximation. Since a single transverse mode is by definition spatially coherent, its phase space is $\lambda/2$. The optical source effective area is A_{em} and the diffraction angle (for a Gaussian mode) is $\lambda_n/\pi w_0$. The temporal coherence time and bandwidth are given by σ_t and $\Delta\omega = 2\pi/\sigma_t$. Consequently, after calculating the total power of a single mode (24), the other optical parameters (radiant intensity, brightness and their spectral counterpart parameters) can also be calculated.

The best choice of beam waist size and position for the transverse radiation modes expansion can only be found by trial and error. However, based on analytical considerations (for Gaussian modes) a sensible first trial choice would be a waist size of harmonic n $w_{\text{Ron}} = w_0/n$ and spot size position at some point within a Rayleigh range $z_R = \pi w_{\text{Ron}}^2/\lambda_n$ from the maximum bunching point.

*(12) The FEL gain for a single mode

$$\frac{\Delta P_q(z)}{P_q(0)} = \frac{1}{2} \left(\frac{\sqrt{\mu_0/\epsilon_0}}{A_{em} P_q(0)} \right)^{1/2} \frac{\bar{a}_w}{\gamma_0 \beta_{z_0}} [JJ]_l I_0 \lambda_w \text{Re} [r_{q_{01}}(z)] \quad (25)$$

This parameter gives the FEL gain of the modulating laser mode. The radiation parameter $r_{q_{01}}(z)$ to be used in (25) corresponds to bunching at the fundamental harmonic and fundamental radiation mode with the beam waist and position of the modulating laser beam

(3). It is calculated from (20,22) with $n = 1$ and $\epsilon_{q_R} = \epsilon_m(r)$.

The super-radiant emission power at the fundamental frequency (Eq. 24 with $n = 1$ and $q = 0, 0$) should in principle be added to (25), but under the assumption of low gain ($\Delta P_q/P_q(0) \ll 1$) its contribution is negligible.

Equation (25) gives the FEL gain in either the small signal (linear gain) or large signal (saturation) regime. In the first case the result should not depend on the choice of modulating laser beam power $P_q(0)$ inserted into the program. As $P_0 = P_m$ increases, saturation is eventually reached and $\Delta P_q/P_q(0)$ diminishes.

*(13) The bunching parameter for off-axis emission.

An alternative approach to the discrete radiation modes expansion is the expansion in terms of continuous radiation modes and particularly plane waves. In analogy to Eq. (11) one may calculate the bunching parameter for emission into angle Θ - $\eta_n(z, \Theta)$.

3. Program Features

The computer code, which is described in more detail in the next chapter, utilizes most of the 3D features of the theoretical model described in the previous chapter. Some generalizations which the model permits have not yet been implemented in the computer code and may be added later.

The 3D features of the code, listed in Table 3, are quite extensive in both the electron beam and radiation field parameters. The model allows arbitrary transverse, angular and energy spread of the electron beam. Describing the various electron distributions in terms of Gaussian functions (which is a particularly good approximation for storage ring beams), the model allows separate focusing in the two transverse (x, y) dimensions with different beam waist spot sizes σ_x , σ_y , and different waist position z_{wx} , z_{wy} . Also, the modulating laser beam (taken to be a fundamental Hermite-Gaussian mode) can have arbitrary x and y focusing parameters (which can be experimentally realized with cylindrical optical components).

Some of the additional improvements of the code, which are presently being implemented or will be added in the future, are allowance for general magnetic field variation of the wiggler, computation of the coherent field amplitude or brightness field at any given observation plane, and computation of FEL gain in the low and high gain regime. The generalization to arbitrary wiggler field variation will allow taking into account random or measured magnet errors, transverse gradient effects, wiggler tapering, and dispersive sections.

Table 3: 3-D Code Model Features

- (1) Initial spatial spread (σ_x, σ_y).
 - (2) Initial angular spread ($\sigma_x, \sigma_y, z_{ewz}, z_{ewy}$).
 - (3) Initial energy spread & tuning ($\sigma_y \gamma_0$).
 - (4) General modulating mode ($w_{0x}, z_{wx}, w_{0y}, z_{wy}$).
 - (5) Excited radiation described in terms of discrete modes (Hermite-Gaussian) / plane waves (angles).
 - (6) Optical parameters: Power/radiant intensity/brightness and the corresponding spectral parameters.
 - (7) Possible extension: Magnet field variation and error.
-

Two different programs are available for calculating the dynamics of the electrons in the wiggler and modulating laser beam fields: An average ponderomotive force model (program PENTOK) and an exact (including longitudinal quiver) model (program PENTOKE). Only the first program has been fully implemented and debugged and requires ~0.1sec computation time per sample electron. The second program may require longer computation time, but may provide more accurate estimates. An improvement in the numerical computation of both programs will be implemented by conversion to parallel and vector processing. This will make it possible to advance in time many sample electrons in parallel, thereby speeding the computation.

4. Technical Description

4.1 General Features

The simulation code for FEL3D consists of two FORTRAN 77 programs, PINPUT, and PENTOK. PINPUT prepares a data file which contains (i) the physical parameters characterizing the wiggler, laser beam, and electron beam, and (ii) the phase space and energy profiles of the electron beam at the entrance of the wiggler. The data file prepared by PINPUT is used by PENTOK, which computes the electron phase space trajectories, bunching, and radiation parameters.

The code for PINPUT was originally written for interactive execution on the VAX cluster at BNL, followed by batch submission of PENTOK to the CDC 7600. Although the code for both PINPUT and PENTOK has been successfully migrated to the IBM 3090, we haven't yet taken advantage of the 3090's screen-oriented display and vector hardware feature. This program is currently underway. Since it requires some amount of recoding, flow charts and other internal details of PINPUT and PENTOK are not being included in the present version of this manual. An updated version will be issued at a subsequent date.

4.2 PINPUT

The purpose of PINPUT is to prepare a data file for PENTOK containing

- (i) the physical parameters which characterize the undulator, laser, and electron beam, and
- (ii) The energy and phase space profiles of the electron beam at the entrance of the undulator.

PINPUT is coded to accept user input interactively. It displays two tables of input parameters, as shown in Tables (4) and (5). The first table to be displayed is:

Table 4: ***FEL Parameter Group*******

1. Lambda_0	2. N_0	3. K
0.10000	22	0.43100E+01
4. Lambda	5. Z_r	6. Z_w
0.53200E-06	0.50000	0.30000E+00
7. Pm [watt]	8. Gamma_0	9. Nmax
0.60000E+08	0.78314E+03	9
Integration parameters:		
10. Zmk step	11. # I steps	12. Acc'y
0.05000	10000	0.000001

At this stage, the user may change any or all of the above parameters by entering the number of the parameter to be changed, and entering the new parameter value.

The parameters in Table (4) are defined as:

1. Lambda_0: Wiggler period (λ_w) in meters.
2. N_0: Number of wiggler periods (N_w).
3. K: RMS wiggler parameter ($\bar{a}_w$) – cf. eqn. (4).
4. Lambda: Modulating laser wavelength in meters.
5. Z_r: Laser Rayleigh length (z_R) in meters – cf. fig. (4); also, see Eqn. (3).
6. Z_w: Laser waist position (z_w) in meters from wiggler entrance – cf. fig (4).
7. Pm: Modulating laser power in watts.
8. Gamma_0: Electron beam energy. If spread in energy is specified, this value represents the center of a Gaussian distribution.
9. Nmax: Highest harmonic (m) of the modulating laser frequency – q table (1).
10. Zmk Step: Integration step size

Fig. 4

11. # I Steps: Total numbers of integration steps taken along the wiggler length. Note that parameters 10 and 11 are not independent, and that specifying any one leads to the other being calculated internally.

12. Acc'y: Accuracy desired of the computation. This parameter is defined by the numerical integration routine which is used to calculate electron trajectories [8].

Table 5: *****Electron Beam Parameter Group*****

Spread in :					
1. X	2. X'	3. Y	4. Y'	5. gamma	
N	N	N	N	N	
6. NX	7. NX	8. NY	9. NY	10. Nga	11. Nphi
1	1	1	1	1	36
12. m	13. SymX	14. SymY			
3	Y	Y			
15. SigX	16. SigX	17. SigY	18. SigY	19. SigGA	
0.1926E-02	0.1157E-03	0.1368E-02	0.1083E-03	0.1768E-03	
20. Xb	21. Xb	22. Yb	23. Yb	24. GAb	
0.2724E-02	0.1636E-03	0.1960E-02	0.1531E-03	0.2500E-03	
25. BetaX	26. EpsX	27. EpsX_s	28. BetaY	29. EpsY	30. EpsY_s
0.1120E+02	0.1500E-06	0.9425E-06	0.1280E+02	0.1500E-06	0.9425E-06

This second parameter group permits one to specify whether there is spread in the transverse direction, or in the beam energy. One has the option of being led through parameters 1 through 30 above one by one, or to change any or all of them directly. If one opts not to change the parameter values directly, PINPUT prompts the user at all stages by displaying the currently stored value of each parameter and for the new value.

Consider, for example, a case in which one wishes to study the effect of beam energy spread, with 20 energies distributed according to a Gaussian with $\sigma_\gamma/\gamma = 10^{-3}$. Since only a few parameters in Table 5 need modification, the user should opt to change variables directly, and enter the following

	<u>Explanation</u>
#5 → Y	"Yes"
#10 → 20	20 energies
#19 → 0.78314	σ_γ computed from parameter #8 in Table 4.

Spread in the transverse dimensions can be handled similarly.

Note that if, for example, one specifies no spread in X and X', the values displayed in Table 5 for X and X' are not used.

The meaning of parameters 1 through 30 in Table 5 follows:

1 to 5: "N" indicates no spread in a given dimension. "Y" indicates that there is spread.

6 to 10: Number of values in a given dimension which are to be sampled according to a Gaussian distribution.

11: Number of phases.

12: Modulating laser harmonic.

13-14: Indicates whether the phase space distribution is symmetric, as explained in sec. 2.3. Choosing symmetry leads to reduced computation time.

15-19: Standard deviation values for spread in a given dimension.

20-30: The parameters in this sub-group allow one to use alternative methods of characterizing the Gaussian spread. The following definitions are relevant

$$20. x_b = \sqrt{2} \sigma_x$$

$$26. \epsilon_x = \sigma_x \sigma'_x$$

$$21. x_{b'} = \sqrt{2} \sigma_{x'}$$

$$27. \epsilon^*_x = 2\pi\epsilon_x$$

$$22. y_b = \sqrt{2} \sigma_y$$

$$28. \beta_y = \sigma_y^2/\epsilon_y$$

$$23. y_{b'} = \sqrt{2} \sigma_{y'}$$

$$29. \epsilon_y = \sigma_y \sigma_{y'}$$

$$24. \gamma_b = \sqrt{2} \sigma_{\gamma}$$

$$30. \epsilon^*_y = 2\pi\epsilon_y$$

$$25. \beta_x = \sigma_x^2/\epsilon_x$$

For any independent choice of parameters characterizing spread, PINPUT computes and displays the corresponding values of x_b , $x'_{b'}$, β_x , ϵ_x , ϵ^*_x , etc.

Program PINPUT also allows the user an alternative way to input the data – by answering questions. If the user decides to use this alternative, he will be asked by the code to give a value for each of the parameters, and will be given the choice of a default value.

4.3 PENTOK: The integration code does not require any user interaction while it is executing. An important practical feature needs to be mentioned. If one runs a case with such realistic features as spread in transverse positions and velocities, and spread in energies, the size of the data files prepared by PENTOK can become extremely large. Note that PENTOK writes two output files with internal filenames OUTPUT and RESULTS, corresponding to logical unit numbers 1 and 3. File "OUTPUT" contains bunching and radiation data, and is typically ~10 Kbytes.

File RESULTS contains the phase space trajectory for each of the transverse positions, velocities, and energy values which are being sampled. If one allows for spread in both transverse directions, as well as in energy, the total number of electron trajectories being computed is obtained by multiplying together parameters 6 thru 11 in Table 5. A typical range of values would be between 10^4 to 10^5 electrons. The storage space required can be computed approximately as 5 Mbytes/ 10^3 electrons.

A fragment of the data files prepared by PENTOK is shown in Figs. (5) and (6). Fig. (5) is taken from the file with internal name OUTPUT, and contains the following data:

(1) The first two lines contain date and time information, and the name of the run which created the file – in this case, the name is "EXAMPLE".

(2) The third line has three integer numbers. The only number of interest here is the last, which is 6. This refers to the number of harmonics for which bunching, radiation, and brightness data is being computed. The 6 harmonics refer to harmonic numbers 1, 3, 5, 7, 9, and 11.

(3) Lines 4 through 7 contain 20 parameters, stored by PENTOK in the array PAR. These number are:

1. Wiggler period λ_w [m]
2. RMS wiggler parameter $\bar{a}_w$.
3. Modulating laser wavelength λ [m]
4. Electron beam energy γ_0 .
5. Laser Rayleigh length z_R [m] – see Fig. 4.
6. Laser waist position z_w [m] – see Fig. 4.
7. Laser waist spot size w_0 [m²].
8. Laser power P_m [watts].
9. Laser electric field [V/m].
10. Floating point conversion of modulating laser harmonic (m).

AUL EXAMPLE	\$			
1 4	5			
0.10000D+00	0.43100D+01	0.53200D-06	0.78314D+03	0.50000D+00
0.30000D+00	0.29098D-03	0.90000D+08	0.71429D+09	0.30000D+01
0.27932D+07	0.54276D+07	0.72740D+07	0.86926D+07	0.98084D+07
0.00000D+00	0.71021D+08	0.71730D+01	0.00000D+00	0.00000D+00
Z (m)	Bunching	Radiation	P-Radiation	
0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00	
0.10000D+00	0.77751D-03	0.37782D-07	0.37782D-07	
0.15000D+00	0.29833D-02	0.12873D-05	0.85817D-06	
0.20000D+00	0.67503D-02	0.12729D-04	0.63643D-05	
0.25000D+00	0.12191D-01	0.68918D-04	0.27567D-04	
0.30000D+00	0.19389D-01	0.26218D-03	0.87395D-04	
0.35000D+00	0.28389D-01	0.79104D-03	0.22601D-03	
0.40000D+00	0.39200D-01	0.20249D-02	0.50624D-03	
0.45000D+00	0.51787D-01	0.45837D-02	0.10186D-02	
0.50000D+00	0.66076D-01	0.94278D-02	0.18856D-02	
0.55000D+00	0.81962D-01	0.17954D-01	0.32644D-02	
0.60000D+00	0.99325D-01	0.32095D-01	0.53492D-02	
0.65000D+00	0.11803D+00	0.54411D-01	0.83709D-02	
0.70000D+00	0.13791D+00	0.88175D-01	0.12596D-01	
0.75000D+00	0.15886D+00	0.13745D+00	0.18327D-01	
0.80000D+00	0.18073D+00	0.20717D+00	0.25896D-01	
0.85000D+00	0.20340D+00	0.30316D+00	0.35666D-01	
0.90000D+00	0.22677D+00	0.43223D+00	0.48026D-01	
0.95000D+00	0.25073D+00	0.60218D+00	0.63388D-01	
0.10000D+01	0.27519D+00	0.82184D+00	0.82184D-01	
0.10500D+01	0.30009D+00	0.11011D+01	0.10487D+00	
0.11000D+01	0.32533D+00	0.14509D+01	0.13190D+00	
0.11500D+01	0.35087D+00	0.18832D+01	0.16375D+00	
0.12000D+01	0.37664D+00	0.24110D+01	0.20092D+00	
0.12500D+01	0.40259D+00	0.30486D+01	0.24389D+00	
0.13000D+01	0.42866D+00	0.38111D+01	0.29316D+00	
0.13500D+01	0.45481D+00	0.47145D+01	0.34923D+00	
0.14000D+01	0.48100D+00	0.57762D+01	0.41258D+00	
0.14500D+01	0.50719D+00	0.70141D+01	0.48373D+00	
0.15000D+01	0.53332D+00	0.84473D+01	0.56315D+00	
0.15500D+01	0.55938D+00	0.10096D+02	0.65133D+00	
0.16000D+01	0.58532D+00	0.11980D+02	0.74873D+00	
0.16500D+01	0.61112D+00	0.14121D+02	0.85583D+00	
0.17000D+01	0.63673D+00	0.16542D+02	0.97306D+00	
0.17500D+01	0.66213D+00	0.19265D+02	0.11009D+01	
0.18000D+01	0.68730D+00	0.22313D+02	0.12396D+01	
0.18500D+01	0.71219D+00	0.25711D+02	0.13898D+01	
0.19000D+01	0.73679D+00	0.29483D+02	0.15517D+01	
0.19500D+01	0.76107D+00	0.33653D+02	0.17258D+01	
0.20000D+01	0.78500D+00	0.38245D+02	0.19123D+01	
0.20500D+01	0.80856D+00	0.43286D+02	0.21115D+01	
0.21000D+01	0.83173D+00	0.48801D+02	0.23238D+01	
0.21500D+01	0.85448D+00	0.54813D+02	0.25495D+01	
0.22000D+01	0.87678D+00	0.61350D+02	0.27886D+01	
Z (m)	Bunching	Radiation	P-Radiation	
0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00	
0.10000D+00	0.68450D-07	0.29284D-15	0.29284D-15	
0.15000D+00	0.26108D-04	0.42874D-10	0.28582D-10	
0.20000D+00	0.10199D-03	0.14773D-08	0.73863D-09	
0.25000D+00	0.19736D-03	0.12799D-07	0.51196D-08	
0.30000D+00	0.30669D-03	0.57102D-07	0.19034D-07	

Fig. 5.