

The Three-Dimensional Free Electron Laser Simulation Code ELFIN

Takeshi NAKAMURA

SPRING-8, Kamigori, Ako-gun, Hyogo 678-12, Japan

1 Introduction

The three-dimensional simulation code of the free electron laser, ELFIN(Electron Laser Field Interaction), was developed. ELFIN simulates an FEL system composed of a monochromatic laser and a continuous electron beam. ELFIN can be applied also to the system in which the bunch length of electrons and pulse length of an input laser are much longer than $N_w \lambda_L$, where N_w is the number of period of a wiggler and λ_L is the wave length of the laser, because they can be seen locally as a continuous electron beam and a monochromatic laser.

ELFIN uses a Fourier transformation method to transform a partial differential equation(PDE) of a laser field to a set of ordinary differential equations(ODEs) with its Fourier coefficients. A kind of predictor-corrector method is used to evolve these ODEs. This scheme eliminate aliasing problems caused by fast longitudinal oscillation of high transverse frequency modes. Such aliasing problem sometimes occurs if we use the naive matrix methods to convert the PDE to ODEs and to solve these ODEs.

2 FEL Equations

ELFIN assumes that the scale of varying of the parameters of electron, laser fields, wiggler field and so on, are much longer than wiggler periods. Hence ELFIN uses the averaged values, such as

$$\bar{Q}(z) = \int_{z-\frac{1}{2}\lambda_w}^{z+\frac{1}{2}\lambda_w} Q(z') dz' \quad (1)$$

where Q is a quantity used in the equations.

The electron position in 6-dimensional space is given by

$$P_i = (\gamma_i, \zeta_i, x_i, y_i, \beta_{x_i}, \beta_{y_i}), \quad P = (P_1, P_2, P_3, \dots, P_{N_p-1}, P_{N_p})$$

where $\zeta = \int_0^z k_w dz + k_L z - \omega_L t$ is the phase in the pondermotive potential and γ, β are the Lorentz factors. The vector potentials of laser field A_L and that of a wiggler field A_w are assumed to have forms,

$$A_L(x, y, z) = \bar{A} |A_L(x, y, z)| \cos(k_L z - \omega_L t + \phi_L(x, y, z)),$$

$$A_w(x, y, z) = -\bar{A} |A_w(x, y, z)| \sin\left(\int_0^z k_w(z') dz' + \phi_w(x, y, z)\right),$$

$$A_w(x, y, z) = A_{w0}(z) \left(1 + \frac{1}{2} h_x(z)^2 x^2 + \frac{1}{2} h_y(z)^2 y^2\right),$$

respectively. ELFIN uses the dimensionless value of them, $a_L(x, y, z) = \frac{e A_L(x, y, z)}{\sqrt{2} m_e c}$ and $a_w(x, y, z) = \frac{e A_w(x, y, z)}{\sqrt{2} m_e c}$ and we assume $|a_L| / |a_w| \ll 1$.

The equation for a laser field is

$$\left\{ -\frac{i}{2k_L} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{\partial}{\partial z} \right\} a_L(x, y, z) = s(P, x, y, z)$$

$$s(P, x, y, z) = \sum_{i=1}^{N_p} s_p(P_i, z) \delta(x - x_i) \delta(y - y_i)$$

$$s_p(P_i, z) = -r_e \sum_{i=1}^{N_p} \frac{1}{\gamma_i} \left\{ |a_{w_i}| [JJ]_i e^{-i(\zeta_i + \phi_{w_i} + \phi_{L_i})} + i a_{L_i} \right\}$$

$$[JJ]_i = J_0(\xi_i) - J_1(\xi_i), \quad \xi_i = \frac{1}{2} |a_{w_i}|^2 / (1 + |a_{w_i}|^2).$$

The values with suffix i is the value for i -th electron.

The equations for electrons are

$$\frac{d\gamma_i}{cdt} = \frac{1}{\gamma_i} |a_{w_i}| |a_{L_i}| [JJ]_i \cos(\zeta_i + \phi_{w_i} + \phi_{L_i})$$

$$\frac{d\zeta_i}{cdt} = k_w - \frac{k_L}{2} (\beta_{x_i}^2 + \beta_{y_i}^2)$$

$$- \frac{k_L}{2\gamma_i^2} \left\{ 1 + |a_{w_i}|^2 - 2 |a_{w_i}| |a_{L_i}| [JJ]_i \sin(\zeta_i + \phi_{w_i} + \phi_{L_i}) \right\}$$

$$\frac{dx_i}{cdt} = \beta_{x_i}, \quad \frac{dy_i}{cdt} = \beta_{y_i}$$

$$\frac{d(\gamma_i \beta_{x_i})}{cdt} = -\frac{a_{w0}^2 h_x^2}{\gamma_i} x_i, \quad \frac{d(\gamma_i \beta_{y_i})}{cdt} = -\frac{a_{w0}^2 h_y^2}{\gamma_i} y_i$$

and these equations for electrons are expressed as

$$\frac{dP_i}{dz} = F(P_i, a_L(x_i, y_i, z), z).$$

We set $cdt = dz$. here and in the following discussion.

3 Periodic Boundary Condition

The periodic boundary condition is imposed on x and y directions as

$$f(x + L_a, y, z) = f(x, y + L_a, z) = f(x, y, z).$$

With this boundary condition, the validity of the choice of the width of the calculation area L_a in (x, y) space can be tested. If the field value at the boundary is too high, we have to increase the width.

4 Fourier Transformation

The (x, y) space of the width L_a is discretized by a square mesh. The coordinate of the mesh points are

$$(x_p, y_q) = (p\Delta x, q\Delta x); \quad p, q = 0, 1, 2, \dots, N_a - 1.$$

The laser field a_L and the source field s on the mesh points are expanded with the Fourier modes

$$u_{lm}(x, y) = \exp\left(i \left(\frac{2\pi}{L_a}\right) (lx + my)\right); \quad l, m = 0, 1, 2, \dots, N_a - 1$$

with Fast Fourier Transformation,

$$\left\{ \begin{array}{l} \tilde{a}_{lm}(z) \\ \tilde{s}_{lm}(z) \end{array} \right\} = \frac{1}{N_a^2} \sum_{p=0}^{N_a-1} \sum_{q=0}^{N_a-1} \left\{ \begin{array}{l} a_L(x_p, y_q, z) \\ s(P, x_p, y_q, z) \end{array} \right\} u_{lm}^*(x_p, y_q)$$

$$a_L(x_p, y_q, z) = \sum_{l=0}^{N_a-1} \sum_{m=0}^{N_a-1} \tilde{a}_{lm}(z) u_{lm}(x_p, y_q).$$

With this, the partial differential equation for the laser field is transformed to the set of ordinary equations

$$\left(\lambda_{lm} + \frac{\partial}{\partial z}\right) \bar{a}_{lm}(z) = \bar{s}_{lm}(z), \quad \lambda_{lm} = \frac{i}{2k_L} \left(\frac{2\pi}{L_a}\right)^2 (l^2 + m^2).$$

The formal solution of these equations are

$$\bar{a}_{lm}(z+\Delta z) = e^{-\lambda_{lm}\Delta z} \left(\bar{a}_{lm}(z) + \int_z^{z+\Delta z} \bar{s}_{lm}(z') e^{\lambda_{lm}z'} dz' \right)$$

5 Interaction of Laser Field and Particles: PIC Method

To introduce the interaction between the laser field and the particles, a Particle-In-Cell method[1] is used. Instead of huge number of electrons, ELFIN uses the moderate number, N_p , of superparticles.

The position of superparticles in the space $(x, y, \beta x, \beta y)$ and γ is generated by a Monte-Carlo method. On the other hand, ξ is generated as $\xi_i = 2\pi(i-1)/N_\xi$, $i=1, 2, \dots, N_\xi$ to establish so-called quiet start and N_ξ is the number of points assigned to ξ coordinate. If ξ is also generated with a Monte-Carlo method, the strong and unphysical spontaneous radiation will be generated.

The laser field $a_L(x, y, z)$ is evaluated on the mesh points and its value at the particle position is obtained as

$$a_L(x_i, y_i, z) = \sum_{p=0}^{N_p-1} \sum_{q=0}^{N_p-1} a_L(x_p, y_q, z) W(x_i - x_p) W(y_i - y_q)$$

And the source field s at the mesh points is evaluated as

$$s(x_p, y_q, z) = \sum_{i=1}^{N_p} s(P_i, z) W(x_i - x_p) W(y_i - y_q).$$

ELFIN uses the following shape function,

$$W(x) = \begin{cases} -\left(\frac{x}{\Delta x}\right)^2 + \frac{3}{4} & (|x| \leq \frac{1}{2}\Delta x) \\ \frac{1}{2}\left|\frac{x}{\Delta x}\right|^2 - \frac{2}{3} & (\frac{1}{2}\Delta x \leq |x| \leq \frac{3}{2}\Delta x) \\ 0 & (\frac{3}{2}\Delta x \leq |x|) \end{cases}.$$

6 Predictor-Corrector Method

To evolve the system, ELFIN uses a kind of predictor-corrector method[2]. To estimate $\bar{a}_{lm}(z + \Delta z)$ using the last equation in section 4, $\bar{s}_{lm}(z)$ in the integral is approximated by the 3-rd order polynomial function

$$\begin{aligned} \bar{s}_{lm}^{(p)}(z) &= \sum_{j=0}^3 C_j^{(p)} u(z)^j, \quad u(z) = \frac{z - z_i}{\Delta z} \\ C_0^{(p)} &= \bar{s}_{lm}(z_n) \\ C_1^{(p)} &= \frac{1}{6}(11\bar{s}_{lm}(z_n) - 18\bar{s}_{lm}(z_{n-1}) + 9\bar{s}_{lm}(z_{n-2}) - 2\bar{s}_{lm}(z_{n-3})) \\ C_2^{(p)} &= \frac{1}{6}(2\bar{s}_{lm}(z_n) - 5\bar{s}_{lm}(z_{n-1}) + 4\bar{s}_{lm}(z_{n-2}) - \bar{s}_{lm}(z_{n-3})) \\ C_3^{(p)} &= \frac{1}{6}(\bar{s}_{lm}(z_n) - 3\bar{s}_{lm}(z_{n-1}) + 3\bar{s}_{lm}(z_{n-2}) - \bar{s}_{lm}(z_{n-3})) \end{aligned}$$

which passes the points $(z_n, \bar{s}_{lm}(z_n))$, $(z_{n-1}, \bar{s}_{lm}(z_{n-1}))$, $(z_{n-2}, \bar{s}_{lm}(z_{n-2}))$ and $(z_{n+1}, \bar{s}_{lm}(z_{n+1}))$.

Then we get the predictors for the laser field,

$$\begin{aligned} \bar{a}_{lm}^{(p)}(z_{n+1}) &= e^{-\lambda_{lm}\Delta z} \left(\bar{a}_{lm}(z_n) + \int_{z_n}^{z_{n+1}} \bar{s}_{lm}^{(p)}(z) e^{\lambda_{lm}z'} dz' \right) \\ &= e^{-\lambda_{lm}\Delta z} \left(\bar{a}_{lm}(z_n) + \sum_{j=0}^3 C_j^{(p)} I_{lm,j} \Delta z \right) \end{aligned}$$

$$\text{where } I_{lm,j} = \int_0^1 u^j e^{(\lambda_{lm}\Delta z)u} du, \quad I_{lm,j+1} = \frac{\partial I_{lm,j}}{\partial (\lambda_{lm}\Delta z)}$$

$$\text{and } I_{lm,0} = \int_0^1 e^{(\lambda_{lm}\Delta z)u} du = \frac{e^{(\lambda_{lm}\Delta z)} - 1}{(\lambda_{lm}\Delta z)}.$$

The predictors for the particles are

$$P_i^{(p)}(z_{n+1}) = P_i(z_n) + F(P_i(z_n), a_L(x_i, y_i, z_n), z_n) \Delta z.$$

The correctors for the particles, which are more plausible than the predictors, are

$$\begin{aligned} P_i(z_{n+1}) &= P_i(z_n) + \frac{1}{2} \{ F(P_i(z_n), a_L(x_i, y_i, z_n), z_n) \\ &\quad + F(P_i^{(p)}(z_{n+1}), a_L^{(p)}(x_i, y_i, z_{n+1}), z_{n+1}) \} \Delta z. \end{aligned}$$

Then, we get $s(P_i(z_{n+1}), x_i, y_i, z_{n+1})$ and its Fourier coefficient $\bar{s}_{lm}(z_{n+1})$. We approximate $\bar{s}_{lm}(z)$ by the 3-rd order polynomial function using this $\bar{s}_{lm}(z_{n+1})$,

$$\begin{aligned} \bar{s}_{lm}^{(c)}(z) &= \sum_{j=0}^3 C_j^{(c)} u(z)^j \\ C_0^{(c)} &= \bar{s}_{lm}(z_n) \\ C_1^{(c)} &= \frac{1}{6}(3\bar{s}_{lm}(z_n) - 6\bar{s}_{lm}(z_{n-1}) + \bar{s}_{lm}(z_{n-2}) - 2\bar{s}_{lm}^{(c)}(z_{n+1})) \\ C_2^{(c)} &= \frac{1}{6}(-2\bar{s}_{lm}(z_n) + \bar{s}_{lm}(z_{n-1}) + \bar{s}_{lm}^{(c)}(z_{n+1})) \\ C_3^{(c)} &= \frac{1}{6}(-3\bar{s}_{lm}(z_n) + 3\bar{s}_{lm}(z_{n-1}) - \bar{s}_{lm}(z_{n-2}) + \bar{s}_{lm}^{(c)}(z_{n+1})) \end{aligned}$$

which passes the points, $(z_n, \bar{s}_{lm}(z_n))$, $(z_{n-1}, \bar{s}_{lm}(z_{n-1}))$, $(z_{n-2}, \bar{s}_{lm}(z_{n-2}))$ and $(z_{n+1}, \bar{s}_{lm}(z_{n+1}))$.

Then we get the more plausible value, correctors,

$$\begin{aligned} \bar{a}_{lm}(z_{n+1}) &= e^{-\lambda_{lm}\Delta z} \left(\bar{a}_{lm}(z_n) + \int_{z_n}^{z_{n+1}} \bar{s}_{lm}^{(c)}(z) e^{\lambda_{lm}z'} dz' \right) \\ &= e^{-\lambda_{lm}\Delta z} \left(\bar{a}_{lm}(z_n) + \sum_{j=0}^3 C_j^{(c)} I_{lm,j} \Delta z \right). \end{aligned}$$

7 Conclusion

The three-dimensional FEL simulation code ELFIN was developed and applied to study several FEL scheme[3,4] including an FEL at the SPring-8 storage ring[5,6], since 1989.

ELFIN had been installed to several machines, from supercomputers; Cray, Hitachi and Fujitsu, to workstations; IBM, HP and Sun. The vectorization is not so high, nearly 90% because of no good algorithm for interpolation of the source at particle points to the mesh points but concurrency has not this problem and can boost the speed of execution.

References

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