U.S. Particle Accelerator School January 25 – February 19, 2021

VUV and X-ray Free-Electron Lasers

Time-dependent 3D FEL Simulations

Petr Anisimov,² Nicole Neveu¹, Dinh C. Nguyen¹

¹ SLAC National Accelerator Laboratory

² Los Alamos National Laboratory









FEL Lattice description





Genesis v2: Lattice file http://genesis.web.psi.ch/Manual/files6.html

outmagfile = 'file_name' delz = 1

version = 1.0

#	header is include	ed.		QF	3.0067E+01	10	100
? VERSION= 1.00 including new format					-3.0000E+01	10	100
? UNITLENGTH= 0.01860 :unit length in header					3.0067E+01	10	100
AW	8.6000E-01	4180	0	QF	-3.0000E+01	10	100
QF	3.0067E+01	5	0	QF	3.0067E+01	10	100
QF	-3.0000E+01	10	100	QF	-3.0000E+01	10	100
QF	3.0067E+01	10	100	QF	3.0067E+01	10	100
QF	-3.0000E+01	10	100	QF	-3.0000E+01	10	100
QF	3.0067E+01	10	100	QF	3.0067E+01	10	100
QF	-3.0000E+01	10	100	QF	-3.0000E+01	10	100
QF	3.0067E+01	10	100	QF	3.0067E+01	10	100
QF	-3.0000E+01	10	100	QF	-3.0000E+01	10	100
QF	3.0067E+01	10	100	QF	3.0067E+01	10	100
QF	-3.0000E+01	10	100	QF	-3.0000E+01	10	100
QF	3.0067E+01	10	100	QF	3.0067E+01	10	100
QF	-3.0000E+01	10	100	QF	-3.0000E+01	10	100
QF	3.006/E+01	10	100	QF	3.0067E+01	5	100
QF	-3.0000E+01	10	100	0X	0.0000E+00	4180	0
	3.000/E+01	10	100	QY	0.0000E+00	4180	0
	-3.0000E+01	10	100	ÂD	0.0000E+00	4180	0
	3.000/E+01	10	100	SL	0.0000E+00	4180	0
	-3.0000E+01	10	100	CX	0.0000E+00	4180	0
	3.000/E+01	10	100	CY	0.0000E+00	4180	0
	-3.0000E+01	10	100	ΔΧ	-0.0000E+00	4180	õ
V NE	2 0000/E+01	10	100	ΔΥ	-0.0000E+00	4180	a a
ųΓ	-3.000000+01	TO	100	A1		4100	0

3





Genesis v2: Lattice file http://genesis.web.psi.ch/Manual/files6.html

outmagfile = 'file_name' = 5

delz

version = 1.0

# he	ader is included			QF	3.0067E+01	2	20
? VE	RSION= 1.00 inc	ludir	QF	-3.0000E+01	2	20	
? UN	ITLENGTH= 0.0930	0 :ur	QF	3.0067E+01	2	20	
AW	8.6000E-01	836	0	QF	-3.0000E+01	2	20
QF	3.0067E+01	1	0	QF	3.0067E+01	2	20
QF	-3.0000E+01	2	20	QF	-3.0000E+01	2	20
QF	3.0067E+01	2	20	QF	3.0067E+01	2	20
QF	-3.0000E+01	2	20	QF	-3.0000E+01	2	20
QF	3.0067E+01	2	20	QF	3.0067E+01	2	20
QF	-3.0000E+01	2	20	QF	-3.0000E+01	2	20
QF	3.0067E+01	2	20	QF	3.0067E+01	2	20
QF	-3.0000E+01	2	20	QF	-3.0000E+01	2	20
QF	3.006/E+01	2	20	QF	3.0067E+01	2	20
QF	-3.0000E+01	2	20	QF	-3.0000E+01	2	20
QF	3.000/E+01	2	20	QF	3.0067E+01	2	20
	-3.0000E+01	2	20	QF	-3.0000E+01	2	20
	3.000/E+01	2	20	QF	3.0067E+01	1	20
	-3.0000E+01 3.0067E+01	2	20	QX	0.0000E+00	836	(
	-3 0007L+01	2	20	QY	0.0000E+00	836	(
	-3.0000E+01	2	20	AD	0.0000E+00	836	(
0F	-3,0000F+01	2	20	SL	0.0000E+00	836	(
0F	3.0067E+01	2	20	CX	0.0000E+00	836	(
0F	-3.0000E+01	2	20	CY	0.0000E+00	836	(
0F	3.0067E+01	2	20	AX	-0.0000E+00	836	(
QF	-3.0000E+01	2	20	AY	-0.0000E+00	836	(
•							

4





Genesis v2: Lattice file <u>http://genesis.web.psi.ch/Manual/files6.html</u>20803

- Header of the file:
 - ? VERSION=1.0
 ? UNITLENGTH='xx'
- Element line:
 - 'XX' 'strength' 'length' 'offset'
- A two-character string, 'XX', indicating the type of structure. Following types are supported:
 - AW Main magnetic field
 - AD Drift section
 - QF Quadrupole strength
 - QX Quadrupole offset in x; QY Quadrupole offset in y
 - SL Solenoid strength
 - CX Corrector strength in x; CY Corrector strength in y





6

Genesis v2: Lattice file simplified

- `maginfile='marie.lat'` supersedes the input file values yet it also depends on
- A real FEL has undulator sectioned!
- Let us introduce the gaps in sections:

```
# header is included
? VERSION= 1.00 including new format
? UNITLENGTH= 0.09300 :unit length in heade
0F
        3.0067E+01
                       1
                            0
AW
        8.6000E-01
                     20
                            1
! LOOP= 19
QF
       -3.0000E+01
                           20
                       2
        8.6000E-01
                      20
                           2
AW
0F
        3.0067E+01
                       2
                           20
AW
        8.6000E-01
                      20
                            2
```

! ENDLOOP

```
gen['xlamd'] = 1.86e-2
gen['awd'] = 0.86
gen['maginfile'] = 'marie.lat'
gen.load_lattice('marie.lat')
```







Genesis Lattice output

? VE	RSION= 1.00 inc	luding	new format		QF	3.0067E+01	1	(
? UN	ITLENGTH= 0.0930	0 :unit	length in	header	QF	-3.0000E+01	2	20
AW	8.6000E-01	20	1		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	-3.0000E+01	2	20
AW	8.6000E-01	20	2		QF	3.0067E+01	2	20
AW	8.6000E-01	20	2		QF	0.0000E+00	20	(
AW	8.6000E-01	20	2		QX	0.0000E+00	857	(

QY	0.0000E+00	857	0	
AD	8.6000E-01	1	0	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	8.6000E-01	2	20	
AD	0.0000E+00	20	0	
			-	

LA-UR-21-20803

7



Phase synchronism in drifts

- We have to fill in the gaps in order to maintain phase synchronism controlled by appropriate phase shifters in actual FELs;
- Sometimes detuning the phase shifter can be used to suppress the fundamental harmonic.







Undulator tapering





Steady-state solution for MaRIE XFEL



- We will explore tapering of the undulator as a way to increase power:
 - wzcoeff(1) starting point;
 - wzcoeff(2) relative change;
 - wzcoeff(3) taper profile.





Undulator (linear taper) – optimization







Undulator (linear taper) – result



12











Phase space distribution (θ, γ)



14











Undulator (quadratic taper) – optimization







Undulator (quadratic taper) – result



























How far can we extend the taper?







How far can we extend the taper?







Genesis 1.3 User Manual Review

http://genesis.web.psi.ch/download/documentation/genesis_manual.pdf



Priority



LA-UR-21-20803

Input/Output Files



Directly imports 6D phase space

Fills up 5D phase space + add phase θ

Local beam parameters + wakes

Global beam parameters + local current

http://genesis.web.psi.ch/download/documentation/genesis_talk.pdf





The Particle Equations



- The independent variable is the distance along the undulator *z*;
- The longitudinal position is replaced by the ponderomotive phase θ of the particle and the transverse momenta are normalized to $m_e c$;
- The transverse motion is solved analytically but these equations depend γ and a higher precision requires to split the pushing of the transverse variables into two half-steps. While the first step relies on γ of the previous iteration, the second uses the updated values of the Runge-Kutta solver for this iteration.

where $\beta_z = \frac{v_z}{c}$, f_c is the coupling JJ factor, a_r and a_u are the scalar, normalized amplitudes of the radiation and undulator field, Ψ is the phase of the radiation field, E_z is the electrostatic field, $b_{x,y}$ are the normalized dipole strengths, $q_{x,y}$ are the quadrupole field strengths and s is the solenoid field strength.





The Field Equations

$$\begin{split} \left[\Delta_{\perp} + \frac{l^2 k^2 (1 + a_u^2)}{\gamma_R^2} \right] E_{z,l} &= i \frac{e c^2 \mu_0 l k (1 + a_u^2)}{\gamma_R^2} \sum_j \delta(\vec{r} - \vec{r_j}) e^{-i l \theta_j} \\ & \left[\Delta_{\perp} + 2i k \frac{\partial}{\partial z} \right] u = i \frac{e^2 \mu_0}{m} \sum_j \delta(\vec{r} - \vec{r_j}) \frac{f_c a_u}{\gamma_j} e^{-i \theta_j} \stackrel{\bullet}{\underset{\text{ele}}{}} \begin{array}{c} \text{On} \\ & \text{ele} \end{array} \end{split}$$

where the resonant energy of the beam is defined as

$$\gamma_R = \frac{\sqrt{k(1+a_u^2)}}{2k_u};$$

where $u = -i a_r e^{i\Psi}$ is the complex representation of the radiation field; note that there is no explicit dependence on *t* in the differential equation. The time dependence is implemented by the slippage mechanism.

- Only the longitudinal component of the electro-static field is taken into account;
- $E_{z,l}$ is the l coefficient of the Fourier expansion in the ponderomotive phase of the electron;
- The transverse profile of the field is discretized on a Cartesian grid with uniform spacing. The Alternating Direction Implicit (ADI) solver guarantees an unconditional stable, fast and memoryefficient method to advance the radiation field one integration step.





Time-dependent Simulation

- *ITDP* = 1 enables the time-dependent simulation;
- *IALL* = 0, *SHOTNOISE* = 1.0 and *PRAD*0 = 0 for SASE simulations;
- The time-window starts at the tail s_0 and ends at the head s_1 ; the required number of slices is $NSLICE = \frac{s_1 s_0}{ZSEP * XLAMDS} > 0$. The first slice has the position s_0 . Therefore NTAIL is $\frac{s_0}{ZSEP * XLAMDS}$.
- GENESIS 1.3 can do only a wild guess about the radiation field which slips into the time-window the tail part of the time-window is physically incorrect. To exclude these slices in the output *IOTAIL* = 0 should be set. The number of suppressed slices is the number of undulator periods of the entire undulator divided by *ZSEP*.





Time-dependent Effects



- GENESIS 1.3 discretizes the radiation field and electron beam in *t*, referring to them as slices;
- Information on the local electron distribution is carried by the radiation field only in the forward direction (slippage) time-dependent simulations rolls over the electron bunch starting from the back;
- Advancing the radiation field is split into two parts: solving the steady-state field equation and copying the field to the next slice;
- Only a single slice of an electron beam and the radiation field over the total slippage length are kept on a compute core.





Graphical representation form Sven's PhD



Schematic order for time-dependent simulations. Due to the slippage the radiation field slices (tilted grey bars) propagate in the forward direction with respect to the electron beam slices (black bars). The integration can either be performed by starting from the end of the bunch and keeping one electron beam slice in memory or from the bunch head with a radiation slice in memory (Method A and B, respectively).





303

Algorithm

Graphical representation



 $DELZ = 0.5, 1, 2, \dots$ such that it can resolve FL, DL, DRL or F1ST;

ZSEP = DELZ, 2DELZ, ... nDELZ, where n is small enough to to avoid collective instabilities of the steady-state field solver per integration step within a single slice.





Genesis simulations - slippage







Genesis simulations







Example of a Gaussian beam profile



- CURLEN = 1e-3 assumes a Gaussian beam profile with an rms length of 1 mm;
- XLAMDS = 5e-6 and ZSEP = 2 define spacing between slices to be equal to $\delta s = 10 \ \mu m$;
- An undulator with NWIG = 200 periods would have $\frac{NWIG}{ZSEP} = 100$ slippage slices;
- A time window starts at $NTAIL = -\frac{3 mm}{10 \mu m}$;

 $10 \ \mu m$

• The total time window of *NSLICE* = 600 contains unphysical slices (100), beam slices (400), slipped out slices (100).





Genesis simulations - slippage

