# FEL Simulations for the European XFEL

# **From GW to TW Radiation Power**



Igor Zagorodnov

**Collaboration Meeting at PAL** 

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#### **Overview**

#### Numerical Methods for FEL Calculations

- □ FEL physics in 1D
- mathematical model in 3D
- numerical methods
- quiet start and shot noise
- time dependent simulations
- problems and challenges
- FEL Simulations for the EXFEL
  - □ SASE for nominal bunch parameters
  - impact of accelerator wakes on SASE
  - self-seeding schemes for TW power
  - strong bunch compresion for TW power
  - undulator tapering in nominal regime
  - harmonic lasing and pSASE





#### **Free Electron Laser**

#### accelerator



# very short and tunable wavelengthextreme short pulses with very high energy

John Madey, Appl. Phys. 42, 1906 (1971)



# **Motivation**



#### Motion of one electron in an undulator





electron trajectory

Field on the axis

 $B_y = -B_0 \sin(k_u z)$ 

$$K = \frac{eB_0}{m_e ck_u} - \text{undulator parameter}$$

 $\gamma$  - electron energy



#### **Energy exchange in FEL**

 $\overline{v}_z < c$  an electron is slower than the EM field





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 $\overline{v}_z < c$  an electron is slower than the EM field



The electron has to be slower exactly by one wave length.

$$\lambda = \frac{\lambda_u}{2\gamma^2} \left( 1 + \frac{K^2}{2} \right)$$



#### Longitudinal equations of motion (1D model)



$$\psi = (k + k_u)z - \omega t, [JJ] \sim 1$$
$$\eta = \frac{\gamma - \gamma_r}{\gamma_r}$$







#### "Low gain" FEL









#### **Microbunching**



experimental evidence of microbunching in Stanford







#### **Field equation**

The EM field variation has to be taken into account

$$\left(\Delta - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) \mathbf{E} = \mu_0 \frac{\partial \mathbf{j}}{\partial t} + \frac{1}{\varepsilon_0} \sqrt{\rho} \qquad \mathbf{E}(z,t) = \Re\left(\tilde{\mathbf{E}}(z,t)\right)$$

#### slowly-varying envelope approximation

$$\tilde{E}_{x}(z,t) = \tilde{E}_{x}(z)e^{i(kz-\omega t)} \qquad \left|\tilde{E}_{x}''(z)\right| << k \left|\tilde{E}_{x}'(z)\right|$$

$$\left[\tilde{V}_{1} + 2ik\left(\frac{\partial}{\partial z} + \frac{1}{c}\frac{\partial}{\partial t}\right)\right]\tilde{E} = ik\mu_{0}c\frac{K}{\gamma}\tilde{j}_{1} \qquad \tilde{E}_{x}'(z) = -\frac{\mu_{0}cK}{4\gamma}\tilde{j}_{1}$$



#### **Longitudinal equations of motion**



**Field equation** 

$$\frac{d}{dz}\tilde{E}_{x}(z) = -\frac{\mu_{0}cK}{4\gamma}\tilde{j}_{1}$$



### "High gain" FEL







# "High gain" FEL





# "High gain" FEL





# "High gain" FEL



#### **3D Effekte**

#### □ transverse beam dynamics

- □ space charge effects
- beam properties (emittance, energy spread etc.)
- □ EM field properties
- undulator properties

FAST FELEX FELS RON FELOS **NUTMEG** FRED3D **GENESIS 1.3** GINGER **MEDUSA SIMPLEX** PERSEO SARAH TDA3D

**FEL codes** 



# **Numerical Methods**

#### **3D FEL codes used at DESY**

	FAST (M.Yurkov)	Genesis 1.3 (S.Reiche)	ALICE (I.Zagorodnov)
Equations of motion	Rung	e-Kutta	leap-frog
EM field	Integral representation	finite-difference, alternating direction	finite difference, Neumann
Boundary conditions	free space	Dirichlet	free space with PML

□ the codes are parallelized

□ a cluster with 360 processors is used



#### **Equations of motion**

$$H^{0}(\mathbf{r},\mathbf{p},t) = c\left(m^{2}c^{2} + (\mathbf{p} + e\mathbf{A})^{2}\right)^{0.5} - e\varphi$$

T.M. Tran, J.S.Wurtele, *Review of free-electronlaser (FEL) simulation techniques*, Phys. Reports 195 (1990) 1

$$\Box \text{ change of independent variable} \qquad \overline{\mathbf{p}}_{\perp} = \frac{\mathbf{p}_{\perp}}{mc}$$
$$H(\mathbf{r}_{\perp}, ct; \overline{\mathbf{p}}_{\perp}, \overline{p}_{t}; z) = -\gamma \left(1 - \frac{1 + |\overline{\mathbf{p}}_{\perp}|^{2} + |\mathbf{a}_{\perp}|^{2} + 2(\overline{\mathbf{p}}_{\perp}, \overline{\mathbf{a}}_{\perp})}{\gamma^{2}}\right)^{0.5} + a_{z} \qquad \mathbf{a} = \mathbf{A} \frac{e}{mc}$$

□ wiggler-period-averaging (helical undulator)

$$\begin{split} \overline{H}(\mathbf{r}_{\perp}, ct; \overline{\mathbf{p}}_{\perp}, \overline{p}_t; z) &= -\gamma \left( 1 - \frac{1 + \left| \overline{\mathbf{p}}_{\perp} \right|^2 + \left| \mathbf{a}_{\perp} \right|^2}{\gamma^2} \right)^{0.5} + a_z \\ \left| \mathbf{a}_{\perp} \right|^2 &= K^2 + 2a_s K \sin(\psi + \varphi_s) + a_s^2 \end{split} \qquad \qquad a_s \equiv \frac{Ee}{mc\omega} \end{split}$$

#### **Equations of motion**

# Iongitudinal



$$\frac{d\gamma}{dz} = -\frac{eK}{m_e c^2 \gamma_r^2} \Re(\tilde{E}e^{i\psi_n}) - \frac{e}{mc^2} E_z$$

#### transverse EM field

longitudinal space charge

□ transverse (slow)

$$\frac{d\,\mathbf{r}_{\perp}}{d\,z} = \frac{\overline{\mathbf{p}}_{\perp}}{\gamma\boldsymbol{\beta}_{z}}$$

$$\frac{d\,\overline{p}_x}{dz} = -\left(\frac{K^2 k_x^2}{\gamma \beta_z} + \frac{eg}{mc}\right) x$$
$$\frac{d\,\overline{p}_y}{dz} = -\left(\frac{K^2 k_y^2}{\gamma \beta_z} - \frac{eg}{mc}\right) y$$



#### **Field equations**

□ transverse field (slowly-varying envelope approximation)

$$E(\vec{r},t) = \tilde{E}(\vec{r},t) \exp\left(i\left(kz - \omega t\right)\right) + c.c. \qquad E = E_x + iE_y$$
$$\left[\nabla_{\perp}^2 + 2ik\left(\frac{\partial}{\partial z} + \frac{1}{c}\frac{\partial}{\partial t}\right)\right]\tilde{E} = ik\mu_0 c\frac{K}{\gamma}\tilde{j}_1$$

 $\Box$  longitudinal space charge (on  $\lambda$  scale)

$$\left(\nabla_{\perp}^{2} - \frac{n^{2}(k+k_{w})^{2}}{\gamma_{z}^{2}}\right)E_{z}^{(n)} = \frac{in(k+k_{w})}{\varepsilon_{0}\gamma_{z}^{2}}\rho^{(n)}$$
$$E_{z}(r,\psi) = \sum E_{z}^{(n)}(r,z)e^{in\psi}$$

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#### **Normalized Equations**

 $\hfill\square$  equations of motion

$$\frac{d\psi}{d\hat{z}} = \hat{C} + \hat{\eta} - \frac{B}{2} \left( \hat{x}^{\prime 2} + \hat{y}^{\prime 2} \right)$$
$$\frac{d\hat{\eta}}{d\hat{z}} = \left| \hat{u} \right| \cos(\psi + \varphi_s) - \hat{E}_z$$

$$\hat{x}'' = -\left(\hat{k}_x^2 + \hat{g}\right)\hat{x}$$
$$\hat{y}'' = -\left(\hat{k}_y^2 - \hat{g}\right)\hat{y}$$

□ field equations

$$\begin{bmatrix} \frac{1}{2iB} \hat{\Delta}_{\perp} + \frac{d}{d\hat{z}} \end{bmatrix} \hat{u} \left( \hat{\mathbf{r}}_{\perp}, \hat{z} \right) = -2a^{(1)} \left( \hat{\mathbf{r}}_{\perp}, \hat{z} \right)$$
$$\hat{E}_{z} = \hat{E}_{z}^{(0)} - \hat{\Lambda}_{p}^{2} \frac{1}{N_{jk}} \sum_{i=1}^{N_{jk}} \left[ \pi \operatorname{sgn}(\psi - \psi_{i}) - (\psi - \psi_{i}) \right]$$

Zagorodnov I., Dohlus M., *Numerical FEL studies with a new code ALICE*, FEL09, Liverpool, 2009.



# **Numerical Methods**

#### **Equations of motion**

□ "leap-frog" scheme for the longitudinal equations

$$\frac{\Psi_{j+0.5} - \Psi_{j-0.5}}{\Delta \hat{z}} = \hat{\eta}_{j} + \hat{C}_{j} - \frac{B}{2} \left( \hat{x}_{j}^{\prime 2} + \hat{y}_{j}^{\prime 2} \right) \qquad j = 1: N_{z}$$
$$\frac{\hat{\eta}_{j+1} - \hat{\eta}_{j}}{\Delta z} = \frac{\hat{u}_{j+1} + \hat{u}_{j}}{2} \cos \left[ \Psi_{j+0.5} + \frac{\varphi_{j+1}^{s} + \varphi_{j}^{s}}{2} \right] + \hat{E}_{z, j+0.5},$$

□ matrix formalism for the transverse equations

$$\begin{pmatrix} \hat{x}_{j+1} \\ \hat{x}'_{j+1} \end{pmatrix} = M_x \begin{pmatrix} \hat{x}_j \\ \hat{x}'_j \end{pmatrix} \qquad \qquad \begin{pmatrix} \hat{y}_{j+1} \\ \hat{y}'_{j+1} \end{pmatrix} = M_y \begin{pmatrix} \hat{y}_j \\ \hat{y}'_j \end{pmatrix}$$



# **Numerical Methods**

#### **Field equation**



#### Perfectly Matched Layer

F. Collino, Journal of Computational Physics 131, 164 (1997)

#### azimuthal expansion

$$\hat{u}(r, z, \varphi) = \sum u^{(m)}(r, z)e^{im\varphi}$$
$$\left[\frac{1}{2iB}\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}-\frac{m^2}{r^2}+\frac{d}{dz}\right]u^{(m)} = -2a^{(1)(m)}$$



#### **Perfectly Matched Layer (PML)**





#### Neumann implicit scheme with PML

$$c_q u_{q+1}^{n+1} + b_q u_q^{n+1} + a_q u_{q-1}^{n+1} = f_q^n$$

The matrix of the system has only three diagonals and we can use the "sweep" method

$$a_{q} = \frac{\Delta z}{4iB} \frac{1}{\tilde{r}_{j}} \frac{\tilde{r}_{j-0.5}}{(\tilde{r}_{j+0.5} - \tilde{r}_{j-0.5})(\tilde{r}_{j} - \tilde{r}_{j-1})} \qquad b_{q} = (1 - a_{q} - c_{q}) - \frac{\Delta z}{iB} \frac{m^{2}}{\tilde{r}_{j}^{2}}$$

$$c_{q} = \frac{\Delta z}{4iB} \frac{1}{\tilde{r}_{j}} \frac{\tilde{r}_{j+0.5}}{(\tilde{r}_{j+0.5} - \tilde{r}_{j-0.5})(\tilde{r}_{j+1} - \tilde{r}_{j})}$$

complex numbers!

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#### **PML performance**





#### **Quiet start in FEL amplifier**





### **Quiet Start and Shot Noise**

#### **Quiet Start ?**





# **Quiet Start and Shot Noise**



The polar form of Box-Muller algorithm (in Genesis, ASTRA) maps the "quiet" uniform distribution in a clustered normal distribution.





$$Y_i = \sigma \sqrt{2} \operatorname{erf}^{-1}(2X_i - 1) + \mu$$

#### **Properties of the normal distribution**

$$\delta = \frac{\left|\sigma_4 - \tilde{\sigma}_4\right|}{\sigma_4} 100\%$$

	N	δ <sub>x</sub> ,	δ <sub>y</sub> ,
		%	%
	7500	1.5	7.5
Genesis v1.0	15000	4.1	4.7
	7500	0.8	1.0
ALICE	15000	0.4	0.4


#### New Genesis v2.0 vs. ALICE





# **Quiet Start and Shot Noise**

#### Convergence



Genesis 1.0: Genesis 2.0: ALICE:

Hammersley and Box-Mueller Hammersley and the inverse error function Sobol and the inverse error function



# **Quiet Start and Shot Noise**

#### Shot noise algorithm



beamlets - a set of 2M particles with the same position  $\mathbf{x}_{\perp} = (x, y, p_x, p_y, \gamma)$ N<sub>b</sub> beamlets with 2M particles each.

$$\left\langle \left| b_k^{(j)} \right|^2 \right\rangle = 0; \quad k = 1: N_b, j = 1: M$$

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# **Quiet Start and Shot Noise**

#### Shot noise algorithm

Small position variations

W.M. Fawley, Phys. Rev. STAB 5 (2002) 070701  $\delta \theta_j = \sum_{m=1}^{m=M} a_m \cos(m\theta_j) + b_m \sin(m\theta_j) \qquad j = 1:2M$   $a_{m,rms} = b_{m,rms} = \sqrt{\frac{2}{N_b m^2}}, \quad m \le M ?!$ 

A more careful analysis for the highest harmonic m=M yields

$$a_{M,rms} = b_{M,rms} = \sqrt{\frac{1}{N_b M^2}}$$



#### Slice parameters are extracted from "Gun-to-Undulator" simulations

$$\gamma \quad \Delta \gamma \quad \varepsilon_x \quad \varepsilon_y \quad \beta_x \quad \beta_y \quad \langle x \rangle \quad \langle y \rangle \quad \langle x' \rangle \quad \langle y' \rangle \quad \alpha_x \quad \alpha_y \quad I$$



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# 



#### ",Slice for slice"

we start from the last slice and track the particles of this slice through the undulator; the radiated EM field is saved.



then we track the next slice in the radiation field of the previous slices



#### **SASE in the European XFEL**



I.Zagorodnov, Ultra-short low charge operation at FLASH and the European XFEL, FEL 2010, Malmö, 2010



#### **Comparison with SPARC FEL experiment**



# **Problems and Challenges**

#### Limitations of the considered FEL model

- □ fast "slalom" motion is not modeled
- only forward propagating field is considered
- macroparticles are locked in the slice with periodic boundary conditions
- only low order harmonics are simulated correctly
- macroscopic space charge, bunch shape changes are not modeled
- narrow frequency bandwidth near the resonance frequency, narrow energy spread



# **Problems and Challenges**

#### "Table-Top-FEL"

M.Fuchs et al, Nature Physics **5**, 826(2009)



strong space charges, large energy spread

fast bunch shape change

- charge or macroparticles redistribution
- macroscopic space charge equation

non-averaged modell



# **Problems and Challenges**

- FEL codes based on averaged equations are checked by experiments
- new FEL schemes (Table Top FEL, Echo-Enabled High-Harmonic Generation etc.) require to consider more physics
- FEL codes based on non-averaged FEL equations, with macroscopic space charge are under development

H.P. Freund, S.G. Biedron, S.V. Milton, IEEE J. Quantum Electron. 36 (2000) 275. (Medusa code)

C.K.W. Nam, P. Aitken, and B.W.J. McNeil, Unaveraged threedimensional modelling of the FEL, FEL 2008, Gyeongju, Korea, 2008



#### Full 3D simulation method (200 CPU, ~10 hours)



W1 -TESLA cryomodule wake (TESLA Report 2003-19, DESY, 2003)

W3 - ACC39 wake (TESLA Report 2004-01, DESY, 2004)

TM - transverse matching to the design optics



#### **Macro-parameters**

Charge	Momentum	Compr.	Momentum	Compr.	Momentum	Total	First	Second
Q,	compaction	in BC <sub>1</sub>	compaction	in BC <sub>2</sub>	compaction	compr.	derivative	derivative
nC	factor in $BC_1$	$C_1$	factor in BC <sub>2</sub>	$C_2$	factor in BC <sub>3</sub>	С	Ζ',	Ζ",
	R <sub>56,1</sub> ,	-	R <sub>56,2</sub> ,	_	R <sub>56,3</sub> ,		[m <sup>-1</sup> ]	$[m^{-2}]$
	[mm]		[mm]		[mm]			1
1	-100	3.5	-54	8	-20	121	0	2000
0.5	-89	3.5	-50	8	-20	217	0	1000
0.25	-78	3.5	-50	8	-20	385	0	1000
0.1	-71	3.5	-50	8	-20	870	0	1000
0.02	-67	3.5	-50	8	-20	4237	0	500

 $E_1 = 130 \,\mathrm{MeV}$   $E_2 = 700 \,\mathrm{MeV}$   $E_3 = 2400 \,\mathrm{MeV}$ 







**Q=500 pC**  $\delta_{_E}$ Phase space Current, emittance, energy spread 10<sup>× 10</sup> 1.2 14.01 5kA 14.005  $-\mathcal{E}_{v}[\mu m]$ 1 14 5 0.8 13.995  $\varepsilon_x$ [µm] -20 20 0.6 0 0.4  $\sigma_{E}$ [MeV] 0.2 -5 -20 20 0 40  $\cap$ -20 20 0 *s* [µm] bunch head *s* [µm]  $\mathcal{E}_{x}^{proj} = 0.7 \, [\mu m]$  $\varepsilon_{v}^{proj} = 2.2 \, [\mu m]$ 

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Parameter	Unit					
Bunch charge	nC	1	0.5	0.25	0.1	0.02
Peak current (gun)	А	43	24	13.5	5.7	1.2
Bunch length (gun, FWHM)	ps	25	22	20	17	17
Slice emittance (gun)	μm	0.8	0.5	0.3	0.21	0.09
Projected emittance (gun)	μm	1	0.7	0.6	0.3	0.1
Compression		114	233	363	877	3833
Peak current	kA	4.9	5.6	4.9	5	4.6
Bunch length (FWHM)	fs	178	72	39	12	2.2
Slice emittance	μm	1	0.7	0.5	0.3	0.2
Projected emittance	μm	3.5	2.2	1.5	0.84	0.26
Slice energy spread	MeV	0.45	0.44	0.6	0.6	0.8
(laser heater off)						





 $W_{\parallel}[kV/m]$ 200 bunch 150 100 50 resistive wake 0 -50 -100 -150 total wake -200 -60 -40 -20 20 40 60 0

*s* [µm]

	Section	Type of element	Number	Loss (V/pC)	%	Spread (V/pC/m)	%	Peak (V/pC/m)	%
► s	SA1	ABS	32	2.389E+03	14	8.717E+02	7	3.451E+03	12
S	SA1	BEL	64	1.342E+03	8	4.476E+02	3	1.803E+03	6
S	SA1	BPME	33	1.780E+03	11	7.243E+02	6	2.598E+03	9
S	SA1	PIPE	33	8.730E+03	53	1.020E+04	80	1.844E+04	62
S	SA1	PIPR	32	7.812E+02	5	1.157E+03	9	2.069E+03	7
S	SA1	PUM	32	3.025E+02	2	2.383E+02	2	5.476E+02	2
S	SA1	RET	32	1.228E+03	7	4.422E+02	3	1.766E+03	6
S	SA1			1.655E+04	100	1.283E+04	100	2.951E+04	100
				1.655E+04	100	1.283E+04	100	2.951E+04	100



#### **Radiation Q=1nC. SASE**



Averaged through 20000 slices

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One shot from different particle distributions

#### Linear undulator tapering



FIG. 2. Normalized output power versus parameter  $\hat{\alpha}$ . Solid:  $\hat{z} = \hat{z}_{sat}(\hat{\alpha})$  (see Fig. 1); dashed:  $\hat{z} = \hat{z}_{sat}(0) = 13$ .

#### PHYSICAL REVIEW SPECIAL TOPICS - ACCELERATORS AND BEAMS 9, 050702 (2006)

#### Self-amplified spontaneous emission FEL with energy-chirped electron beam and its application for generation of attosecond x-ray pulses

E. L. Saldin, E. A. Schneidmiller, and M. V. Yurkov Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany (Received 17 March 2006; published 3 May 2006)  $\hat{\alpha}_{opt} = 0.25$  $\hat{C}(\hat{z}) = \hat{b}\hat{z}$  $\hat{b}_{opt} = 0.5\alpha_{opt}$  $\hat{C}(\hat{z}) = 0.125\hat{z}$ 

$$\frac{dK}{dz} \approx \frac{1}{kK} \left( 2k_u \gamma \frac{d\gamma}{dz} - 0.5 \left( k_u \rho \gamma \right)^2 \right)$$



#### **Linear undulator tapering**









#### Mismatch and wake Q=250 pC





#### **Radiation Q=250 pC**





#### Mismatch and wake Q=20 pC





#### **Radiation Q=20 pC**





#### **Slice parameters for SASE simulations**

Slice parameters are extracted from S2E simulations for SASE simulations



#### Radiation energy statistics (1-25-120 runs)



Charge, nC	1	0.25	0.02
Mean radiation energy, mJ	1-4	1-2	0.1-0.4
Pulse radiation width (FWHM), fs	25-50	10-20	1-2



#### Radiation energy statistics Q=20 pC (120 runs)









#### Summary

Bunch charge, nC	1	0.25	0.02		
Wavelength, nm	0.1				
Beam energy, GeV	14				
Peak current, kA	~ 5				
Slice emmitance,mm-mrad	1	0.5	0.2		
Saturation length, m	85	60	45		
Energy in the rad. pulse, mJ	1-4	1-2	0.1-0.4		
Radiation pulse duration FWHM, fs	25-50	10-20	1-2		
Averaged peak power, GW	10-50	10-100	50-150		
Spectrum width, %		0.15-0.3	0.18-0.5		


#### Impedance Budget (list of elements)

El.type	Num.	Loss (kV/nC)	% Sp	oread (kV/nC)	%	Peak(kV/nC)	%
BPMF	4	4.075E+01	0	1.858E+01	0	5.804E+01	0
COL	7	6.725E+03	19	3.373E+03	22	1.058E+04	21
кіск	3	3.645E+03	10	1.459E+03	9	5.283E+03	10
PIP20	1	5.116E+03	14	3.661E+03	24	8.959E+03	18
PUMCL	78	5.605E+02	2	2.363E+02	2	7.946E+02	2
CAV	808	1.481E+04	42	8.842E+03	57	2.814E+04	56
CAV3	8	8.084E+01	0	3.010E+01	0	1.117E+02	0
FLANG	500	1.330E+03	4	5.610E+02	4	1.886E+03	4
TDS	8	1.507E+03	4	7.348E+02	5	2.174E+03	4
OTRB	8	1.584E+02	0	7.251E+01	0	2.254E+02	0
STEP1	1	3.010E+00	0	5.969E-01	0	3.441E+00	0
BPMA	107	5.654E+02	2	2.896E+02	2	8.670E+02	2
OTRA	12	3.078E+02	1	1.274E+02	1	4.494E+02	1
BPMC	56	4.431E+01	0	2.138E+01	0	6.805E+01	0
BPMR	26	2.993E+02	1	1.304E+02	1	4.501E+02	1
DCM	4	1.644E+01	0	7.479E+00	0	2.315E+01	0
BPMB	27	5.744E-02	0	1.587E-01	0	6.023E-01	0
BAM	5	3.319E+00	0	1.494E+00	0	4.768E+00	0
TORA	3	3.147E+01	0	1.609E+01	0	4.763E+01	0
TORAO	6	1.856E+02	1	7.684E+01	0	2.700E+02	1
		3.530E+04	100	1.540E+04	100	5.037E+04	100

### Accelerator wakes. Q=1nC





#### Accelerator wakes. Q=1nC



#### "Artificially" matched beam. Q=1nC



With full accelerator and undulator wake

$$\left(\frac{dK}{dz}\right)_{opt} = -4.8 \cdot 10^{-5} \,\mathrm{m}^{-1}$$



#### Beam matched in the peak current. Q=1nC





### Beam matched in the peak current. Q=1nC



El.type	Num.	Loss (kV/nC)	% Sp	read (kV/nC)	%	Peak (kV/nC)	%
BPMF	4	6.150E+01	0	2.891E+01	0	8.933E+01	0
COL	7	2.283E+04	32	1.022E+04	31	3.452E+04	35
кіск	3	7.893E+03	11	3.100E+03	9	1.052E+04	11
PIP20	1	1.652E+04	23	8.512E+03	26	2.730E+04	27
PUMCL	78	1.103E+03	2	4.743E+02	1	1.574E+03	2
CAV	808	1.574E+04	22	9.440E+03	29	2.987E+04	30
CAV3	8	9.280E+01	0	3.590E+01	0	1.316E+02	0
FLANG	500	2.619E+03	4	1.126E+03	3	3.736E+03	4
TDS	8	2.506E+03	4	1.229E+03	4	3.677E+03	4
OTRB	8	2.428E+02	0	1.137E+02	0	3.510E+02	0
STEP1	1	3.825E+00	0	6.815E-01	0	4.293E+00	0
BPMA	107	7.317E+02	1	4.231E+02	1	1.265E+03	1
OTRA	12	1.698E+02	0	8.118E+01	0	2.474E+02	0
BPMC	56	7.912E+01	0	4.531E+01	0	1.348E+02	0
BPMR	26	1.523E+02	0	7.506E+01	0	2.241E+02	0
DCM	4	2.533E+01	0	1.160E+01	0	3.612E+01	0
врмв	27	1.247E-01	0	1.976E-01	0	7.440E-01	0
BAM	5	4.474E+00	0	2.180E+00	0	6.820E+00	0
TORA	3	4.681E+01	0	2.515E+01	0	7.275E+01	0
TORAO	6	1.107E+02	0	5.175E+01	0	1.598E+02	0
		7.063E+04	100	3.285E+04	100	1.000E+05	100

#### Accelerator wakes. Q=250 pC.









### Beam matched in the peak current. Q=250 pC





## Beam matched in the peak current. Q=250 pC



![](_page_80_Picture_4.jpeg)

El.type	Num.	Loss (kV/nC)	% Sp	read (kV/nC)	%	Peak (kV/nC)	%
BPMF	4	1.028E+02	0	4.822E+01	0	1.602E+02	0
COL	7	1.040E+05	57	8.502E+04	83	2.999E+05	75
кіск	3	3.017E+04	17	1.808E+04	18	6.233E+04	16
PIP20	1	1.975E+04	11	1.126E+04	11	3.789E+04	9
PUMCL	78	2.666E+03	1	1.237E+03	1	4.514E+03	1
CAV	808	1.670E+04	9	9.809E+03	10	3.109E+04	8
CAV3	8	9.994E+01	0	3.871E+01	0	1.424E+02	0
FLANG	500	6.328E+03	3	2.937E+03	3	1.072E+04	3
TDS	8	4.847E+03	3	2.648E+03	3	8.072E+03	2
OTRB	8	4.257E+02	0	2.010E+02	0	6.740E+02	0
STEP1	1	4.406E+00	0	7.830E-01	0	4.846E+00	0
BPMA	107	7.840E+02	0	4.502E+02	0	1.352E+03	0
OTRA	12	3.035E+02	0	1.468E+02	0	4.863E+02	0
BPMC	56	8.884E+01	0	5.119E+01	0	1.636E+02	0
BPMR	26	3.036E+02	0	1.547E+02	0	5.074E+02	0
DCM	4	4.672E+01	0	2.190E+01	0	7.487E+01	0
врмв	27	1.755E-01	0	2.488E-01	0	7.636E-01	0
BAM	5	5.023E+00	0	2.364E+00	0	7.486E+00	0
TORA	3	6.546E+01	0	3.326E+01	0	9.760E+01	0
TORAO	6	1.989E+02	0	9.429E+01	0	3.173E+02	0
		1.810E+05	100	1.019E+05	100	4.004E+05	100

## Accelerator wakes. Q=20 pC

![](_page_81_Figure_3.jpeg)

![](_page_81_Picture_4.jpeg)

#### Accelerator wakes. Q=20 pC

![](_page_82_Figure_2.jpeg)

![](_page_82_Picture_4.jpeg)

#### Beam matched in the peak current. Q=20 pC

![](_page_83_Figure_2.jpeg)

![](_page_83_Picture_3.jpeg)

## Beam matched in the peak current. Q=20 pC

![](_page_84_Figure_2.jpeg)

![](_page_84_Figure_3.jpeg)

#### FWHM=0.58%

FWHM=1.0%

![](_page_84_Picture_7.jpeg)

#### Summary

	A applanator walta	Bunch charge, nC			
	Accelerator wake	1	0.25	0.02	
Energy in the radiation pulse	x1	9	2.3	0.46	
at $z=175$ m, mJ	x4	8	2.3	0.44	
	x8	6	2.3	0.43	
	x1	0.14	0.29	0.55	
Spectrum width at z=85m, %	x4	0.23	0.30	0.58	
	x8	0.6	0.38	1.0	

We have considered only the **longitudinal** wake in a quite coarse model (adding the accelerator wake at the undulator entrance). The **transverse** wakes are neglected.

![](_page_85_Picture_4.jpeg)

![](_page_86_Picture_1.jpeg)

![](_page_86_Picture_3.jpeg)

#### **Requirements for bio-imaging**

- the imaging method "diffraction before destruction" requires pulses containing enough photons to produce measurable diffraction patterns and short enough to outrun radiation damage
- the higher is intensity, the stronger is the diffracted signal and the higher resolution can be achieved
- bio-imaging capabilities can be obtained by reducing the pulse duration to 10 fs or less and simultaneously increasing the number of photons per pulse to about 10<sup>14</sup>
- $\Box$  Key metric is photon power. Ideally ~ 10 TW (10<sup>14</sup> photons at ~3.5 keV is
  - ~ 60 mJ and in 10 fs ~ 6 TW)

E.Saldin , Perspectives of imaging of single macromolecular complexes at the European XFEL, CFEL Seminar, Hamburg, 8.05. 2013

### **Calculated scattering from a single molecule**

It is confirmed by simulations that, with 10<sup>14</sup> photons per 10 fs pulse at 3.5 keV photon energy in a 100 nm focus, one can achieve diffraction to the desired resolution. This is exemplified using photosystem-I membrane protein as a case study

![](_page_88_Picture_3.jpeg)

E.Saldin , Perspectives of imaging of single macromolecular complexes at the European XFEL, CFEL Seminar, Hamburg, 8.05. 2013

Simulated diffraction pattern

#### Courtesy of S. Serkez and O. Yefanov

![](_page_88_Picture_7.jpeg)

#### Self-seeding and undulator tapering

According to the present design of EXFEL, SASE power saturates at ~ 50 GW. This is very far from 10 TW-power level required for imaging of single bio-molecules.

There is cost-effective way to improve the output power:

Self-seeding and undulator tapering greatly improves FEL efficiency

Cost of self-seeding setup with single crystal monochromator is ~ 2 MEUR. Undulator tapering is based on the used the baseline tunable gap undulator and can be implemented without additional cost.

E.Saldin , Perspectives of imaging of single macromolecular complexes at the European XFEL, CFEL Seminar, Hamburg, 8.05. 2013

![](_page_89_Picture_8.jpeg)

## **Strong Compression for Q=1 nC**

![](_page_90_Figure_2.jpeg)

#### Current, emittance, energy spread

![](_page_90_Figure_4.jpeg)

![](_page_90_Picture_6.jpeg)

#### **Aluminum Foil in BC**

![](_page_91_Figure_2.jpeg)

#### Fig. 2. The slotted foil at chicane center generates a narrow, unspoiled beam center

DESY

## **Aluminum Foil in BC**

![](_page_92_Figure_2.jpeg)

Fig. 3. Left plot: Current profile after BC3 without foil. Right plot: Longitudinal phase space distribution of the particles after BC3, with foil. The simulation includes multiple Coulomb scattering in a  $2\mu$ m thin aluminum foil with a slot width of 0.7 mm.

![](_page_92_Picture_4.jpeg)

## **Aluminum Foil in BC**

![](_page_93_Figure_2.jpeg)

Fig. 4. Left plot: Vertical normalized emittance as a function of the position inside the electron bunch after BC3. The grey dashed curve is from particle tracking without foil. The black dashed curve is from particle tracking with foil. Right plot: Horizontal emittance as a function of the position inside the electron bunch after BC3. The grey dashed curve is from particle tracking without foil. The black dashed curve is from particle tracking with foil. (In both plots we removed 6 % of strongly scattered particles from the analysis.)

![](_page_93_Picture_5.jpeg)

### **Self-seeding**

![](_page_94_Figure_2.jpeg)

Fig. 5. Scheme for a 10 TW-power level undulator source. Self-seeding and undulator tapering greatly improve the FEL efficiency. X-ray pulse length control is obtained using a slotted foil in the last bunch compressor. The magnetic chicane accomplishes three tasks by itself. It creates an offset for single crystal monochromator, it removes the electron microbunching produced in the upstream undulator, and it acts as a magnetic delay line.

![](_page_94_Picture_4.jpeg)

![](_page_95_Figure_1.jpeg)

#### Courtesy V.Kocharyan

Fig. 9. Power distribution and spectrum of the SASE x-ray pulse at the exit of the first undulator.

![](_page_95_Figure_4.jpeg)

Fig. 10. Power distribution and spectrum of the SASE x-ray pulse at after the wake monochromator. The seed pulse is indicated by an arrow in the left plot.

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![](_page_96_Figure_1.jpeg)

Fig. 12. Power distribution and spectrum of the output radiation pulse. The self--seeded line 1 is compared with the SASE line 2, showing the advantages of our method. The SASE spectrum is magnified of a factor 100, to make it visible in comparison with the self-seeded spectrum.

![](_page_96_Picture_3.jpeg)

#### **Self-seeding and tapering**

![](_page_97_Figure_2.jpeg)

Fig. 11. Taper configuration for high-power mode of operation at 0.35 nm.

![](_page_97_Figure_4.jpeg)

Fig. 13. Energy of the seeded FEL pulse as a function of the distance inside the output undulator.

![](_page_97_Picture_6.jpeg)

## **Strong Bunch Compresion for TW Power**

### Strong compression and undulator tapering

![](_page_98_Figure_2.jpeg)

![](_page_98_Figure_3.jpeg)

DESY 13-109

June 2013

Svitozar Serkez<sup>*a*</sup>, Vitali Kocharyan<sup>*a*</sup>, Evgeni Saldin<sup>*a*</sup>, Igor Zagorodnov<sup>*a*</sup>, Gianluca Geloni<sup>*b*</sup>, and Oleksander Yefanov<sup>*c*</sup>

Extension of SASE bandwidth up to 2% as a way to increase the efficiency of protein structure determination by x-ray nanocrystallography at the European XFEL

#### DESY 13-138

#### August 2013

Svitozar Serkez<sup>a</sup>, Vitali Kocharyan<sup>a</sup>, Evgeni Saldin<sup>a</sup>, Igor Zagorodnov<sup>a</sup>, Gianluca Geloni<sup>b</sup>

#### Proposal to generate 10 TW level femtosecond x-ray pulses from a baseline undulator in conventional SASE regime at the European XFEL

![](_page_98_Picture_13.jpeg)

# **Strong Bunch Compresion for TW Power**

## Strong compression and undulator tapering

![](_page_99_Figure_2.jpeg)

Fig. 7. Evolution of the output energy in the photon pulse and of the variance of the energy fluctuation as a function of the distance inside the output undulator, with tapering. Grey lines refer to single shot realizations, the black line refers to the average over a hundred realizations.

![](_page_99_Picture_4.jpeg)

# **Strong Bunch Compresion for TW Power**

## Strong compression and undulator tapering

![](_page_100_Figure_2.jpeg)

Fig. 5. Power and spectrum produced in the SASE mode at saturation with undulator tapering. Grey lines refer to single shot realizations, the black line refers to the average over a hundred realizations.

![](_page_100_Picture_4.jpeg)

# **Non-linear Tapering in Nominal Regime**

#### Current and taper for Q=250 pC

![](_page_101_Figure_2.jpeg)

![](_page_101_Picture_3.jpeg)

## **Non-linear Tapering in Nominal Regime**

## **SASE ALICE and Genesis (v. 2.0) with intersections, quantum fluctations, taper and wake**

![](_page_102_Figure_2.jpeg)

Igor Zagorodnov | Collaboration Meeting at PAL | 2-6. August 2013 | Seite 103

DES

## **Non-linear Tapering in Nominal Regime**

## **SASE ALICE and Genesis (v. 2.0) with intersections, quantum fluctations, taper and wake**

![](_page_103_Figure_2.jpeg)

![](_page_103_Picture_3.jpeg)

#### B. W. J. McNeil et al., Phys. Rev. Lett. 96, 084801 (2006).

E. A. Schneidmiller and M. V. Yurkov, Phys. Rev. ST Accel. Beams 15, 080702 (2012).

![](_page_104_Figure_3.jpeg)

#### A possible upgrade of FLASH for harmonic lasing down to 1.3 nm

E.A. Schneidmiller and M.V. Yurkov

![](_page_104_Picture_6.jpeg)

![](_page_105_Figure_1.jpeg)

Fig. 4. Pulse energy versus magnetic length of the undulator for the fundamental (solid) and the 3rd harmonic (dash). Electron beam and undulator parameters are given in Table 1. Phase shifters are located after every 0.5 m long section of the undulator. The phase shift is  $4\pi/3$  after sections 1-4, 6-9, 11-13, 18, 23, 39-49, and  $2\pi/3$  after sections 5, 10, 14-17, 19-22, 24-27.

![](_page_106_Figure_1.jpeg)

FIG. 8. An example for the European XFEL. Averaged peak power for the fundamental harmonic (solid) and the third harmonic (dash) versus magnetic length of SASE1 undulator. The wavelength of the third harmonic is 0.2 Å (photon energy 62 keV). The fundamental is disrupted with the help of phase shifters installed after 5 m long undulator segments. The phase shifts are  $4\pi/3$  after segments 1–8 and 21–26, and  $2\pi/3$  after segments 9–16. Simulations were performed with the code FAST.

![](_page_106_Picture_4.jpeg)

![](_page_107_Figure_1.jpeg)

FIG. 7. Averaged peak power for the fundamental harmonic (solid) and the third harmonic (dash) versus geometrical length of the LCLS undulator (including breaks). The wavelength of the third harmonic is 0.5 Å (photon energy 25 keV). Beam and undulator parameters are in the text. The fundamental is disrupted with the help of the spectral filter (see the text) and of the phase shifters. The phase shifts are  $4\pi/3$  after segments 1–5 and 17–22, and  $2\pi/3$  after segments 6–10 and 23–28. Simulations were performed with the code FAST.

![](_page_107_Picture_4.jpeg)
## Harmonic Lasing and pSASE

E. A. Schneidmiller and M. V. Yurkov, Phys. Rev. ST Accel. Beams 15, 080702 (2012).

DESY 13-135

July 2013

Svitozar Serkez<sup>a</sup>, Vitali Kocharyan<sup>a</sup>, Evgeni Saldin<sup>a</sup>, Igor Zagorodnov<sup>a</sup>, Gianluca Geloni<sup>b</sup>

Purified SASE undulator configuration to enhance

the performance of the soft x-ray beamline at the

D. Xiang, Y. Ding, Z. Huang and H. Deng., Phys. Rev. ST AB 16, 010703 (2013).



Fig. 2. The actual pSASE undulator configuration proposed for the SASE3 beamline, which is expected to operate in the photon energy range between 1.3 keV and 3 keV.

## Harmonic Lasing and pSASE



## Harmonic Lasing and pSASE



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