Computational Needs for XFELs

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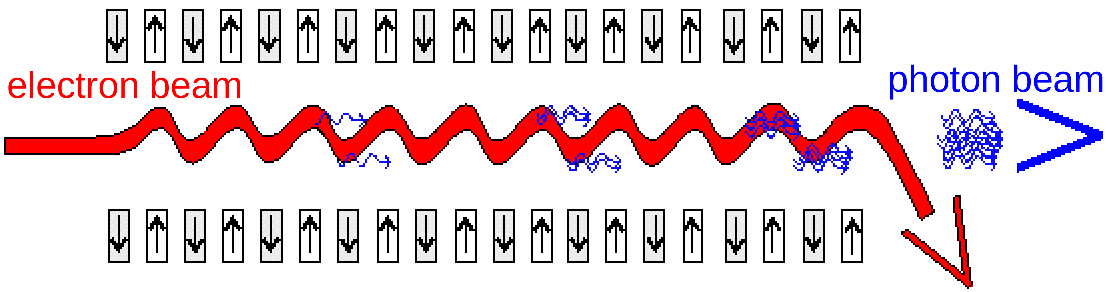
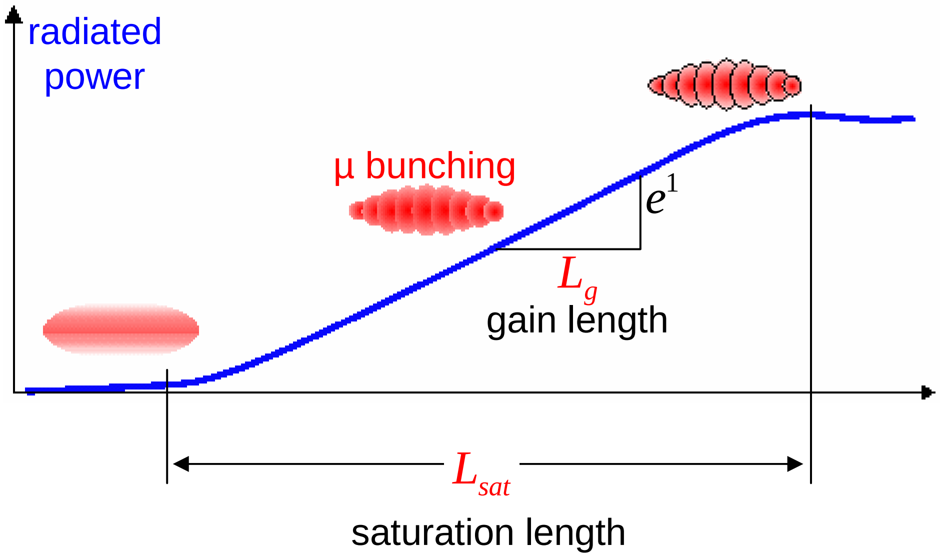
TOC

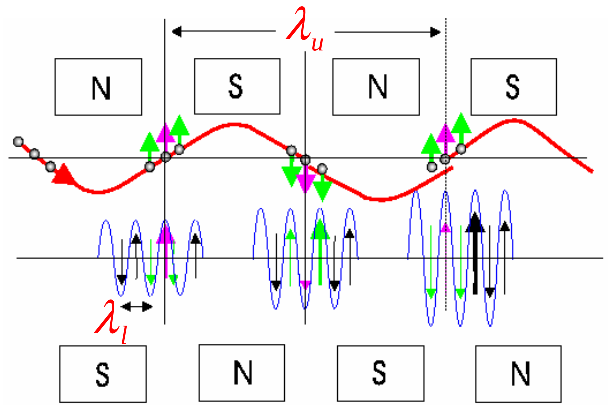
about FELs: SASE XFEL



Self **A**mplifying **S**pontaneous **E**mission



resonant interaction:



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

what are the physical challenges?

resonance energy

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

small gain length

$$L_g \propto \sqrt[3]{\frac{2mc}{\mu_0 e}\cdot\frac{\gamma^3\lambda_u}{K^2}\cdot\frac{\sigma_r^2}{\hat{I}}}$$ current density

(1d theory)

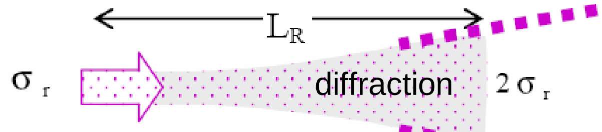
resonance condition

emittance & optics

$$\lambda_l = \frac{\lambda_u}{2(\gamma_0+\delta\gamma)^2}\left(1+\frac{K^2}{2}\right)+\frac{\lambda_u}{2}\left(x'^2+y'^2\right)$$

energy spread

overlap electron – photon beam $\sigma_r \approx \sigma_{r,l}$ $\quad L_g \approx L_r$



$$\sigma_{r,l} \approx \sqrt{L_r\lambda_l/\pi}$$

what are the physical challenges?

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

$K \propto 1$

$\lambda_u \propto \mathrm{cm}$

$\lambda_l \approx 10\ \mathrm{nm} \rightarrow E \propto \mathrm{GeV}$

FLASH 13nm@690MeV

$\lambda_l \approx 0.1\ \mathrm{nm} \rightarrow E \propto 10\,\mathrm{GeV}$

LCLS 0.15nm@14GeV
Europ. XFEL 0.1@17GeV

$L_u > L_{sat} \propto 10 L_g$ $\propto 100\ \mathrm{m}$

undulator length
FLASH ~ 30m
LCLS ~ 120m
Europ. XFEL ~ 200m

$$L_g \propto \sqrt[3]{\frac{2mc}{\mu_0 e} \cdot \frac{\gamma^3 \lambda_u}{K^2} \cdot \frac{\sigma_r^2}{\hat{I}}}$$

(1d theory)

current $\hat{I} \approx 1 \cdots 10\ \mathrm{kA}$

FLASH ~ 1…2 kA
Europ. XFEL ~ 5 kA

$\sigma_r \propto \sqrt{L_g \lambda_l}$

FLASH ~ 100µm
LCLS, E-XFEL ~ 30µm

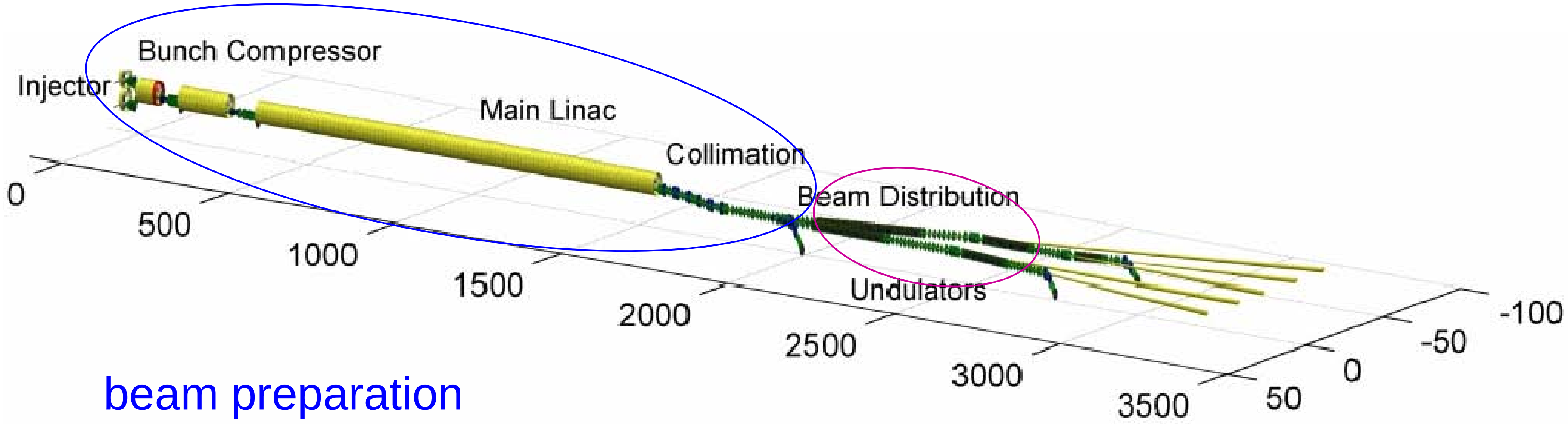
emittance $\varepsilon < \dfrac{\lambda_l}{4\pi}$

normalized emittance $\varepsilon_n \approx 1\,\mu\mathrm{m}$

bandwidth ↔ energy spread $\Delta E / E \propto \lambda_u / L_g$

FLASH, XFEL ~ 1 MeV

accelerator and SASE FEL



beam preparation

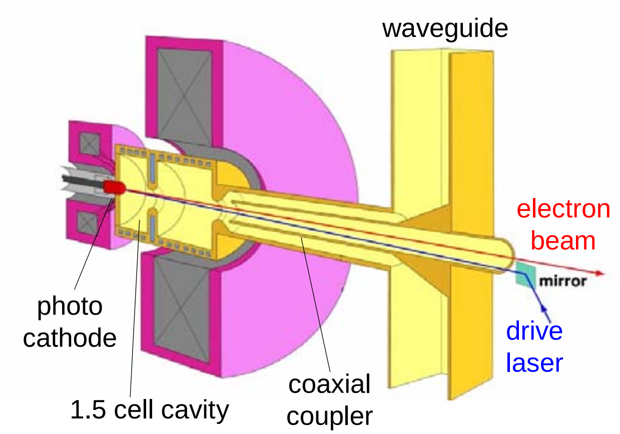
- gun
- injector
- BC system
- linac

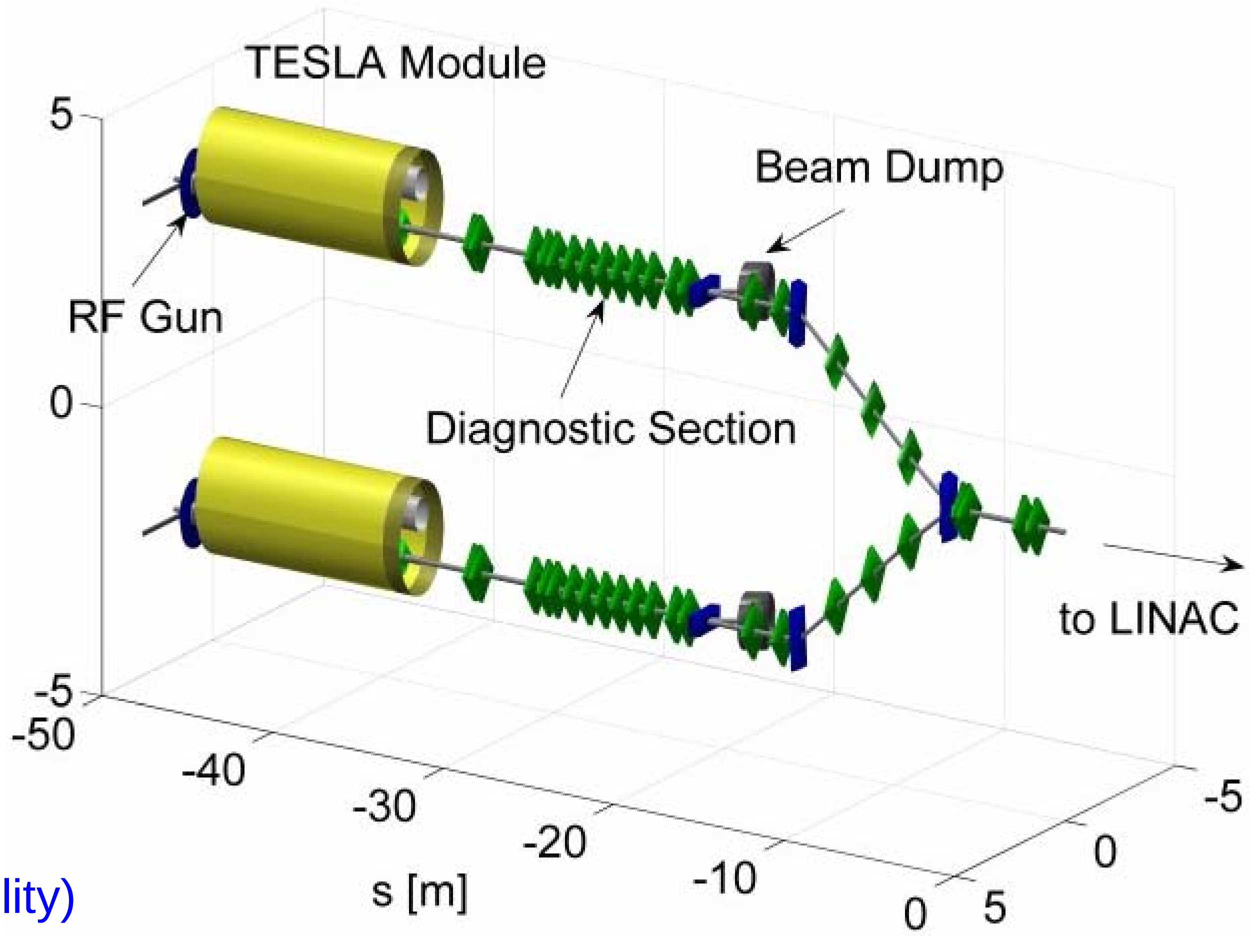
FEL & SASE

gun & injector

~ 50 A; ~ 130 MeV

RF Gun

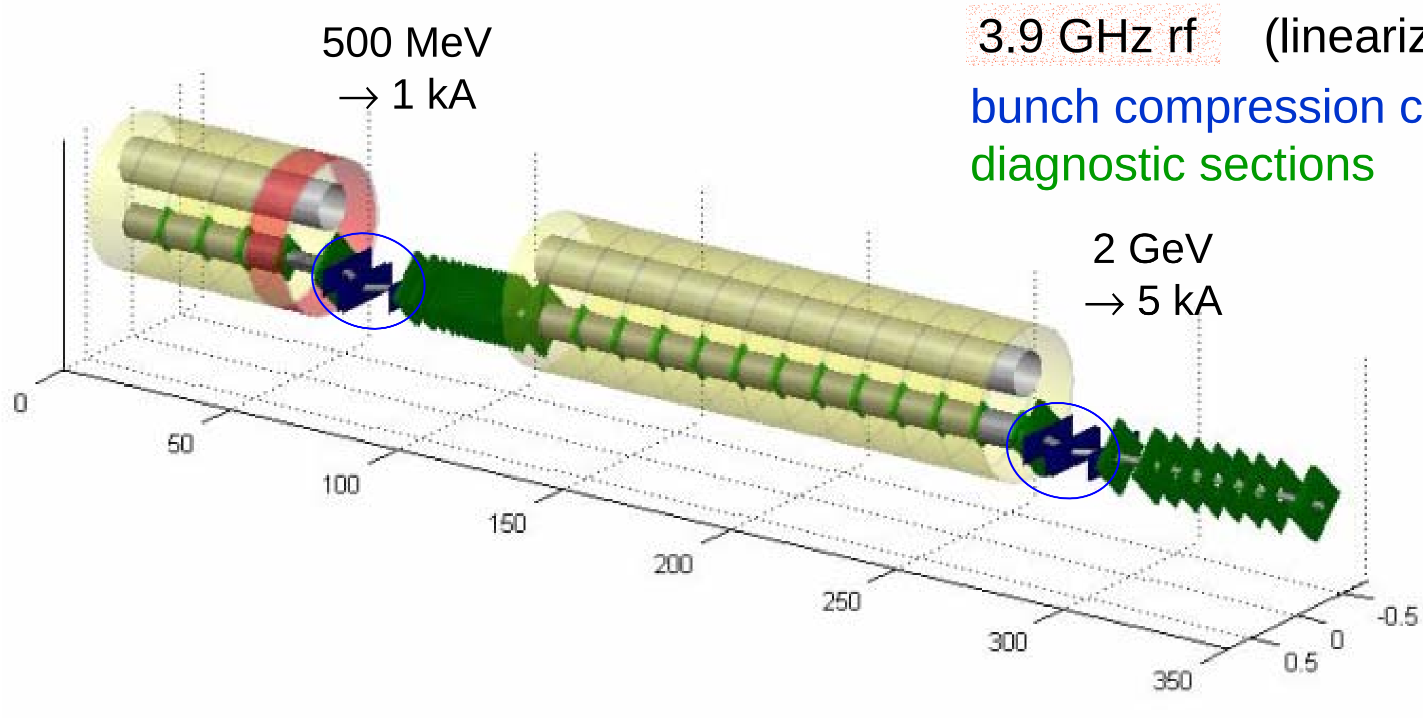




drive laser
external fields (field stability)
space charge effects

bunch compression system

1.3 GHz rf
3.9 GHz rf (linearization)
bunch compression chicanes
diagnostic sections



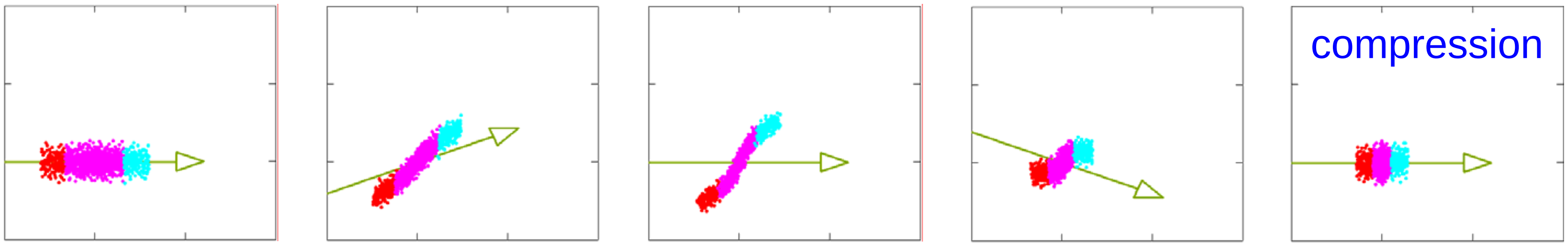
external fields (field stability)
space charge effects
coherent synchrotron radiation
wakes

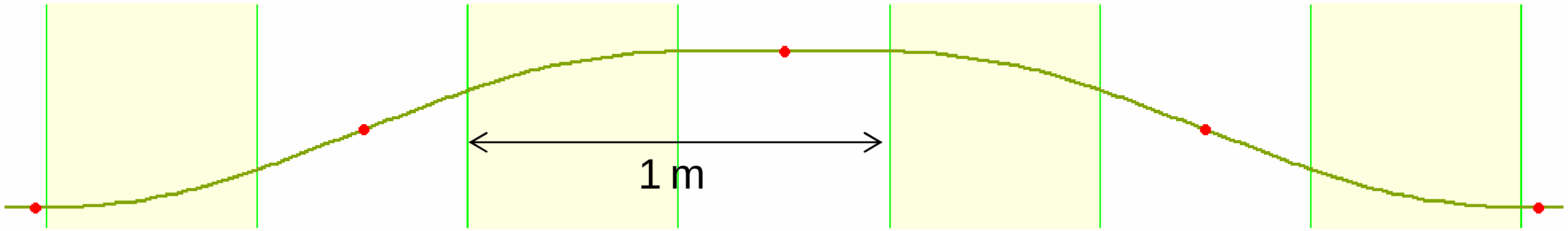
… CSR effects

shape variation

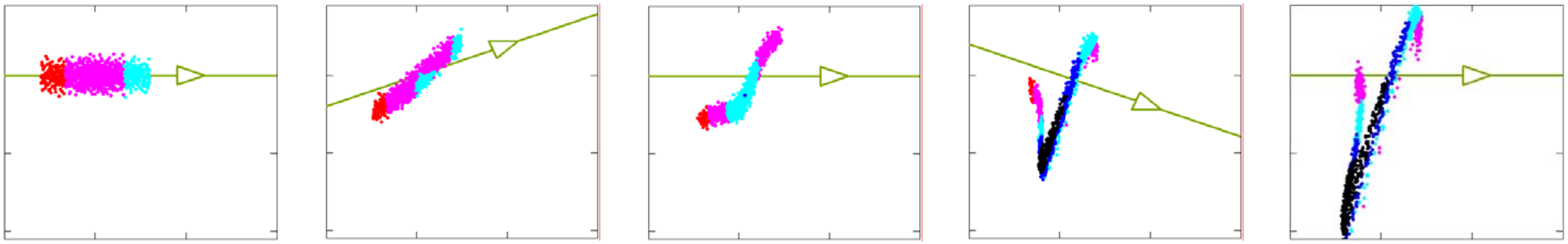
top view (horizontal plane), color = energy

without self-interaction





with self-interaction



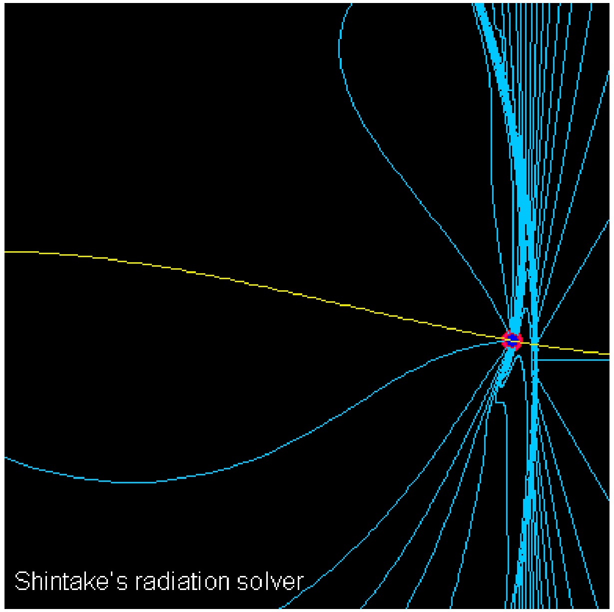
emittance growth

CSR effects

radiation effects

overtaking

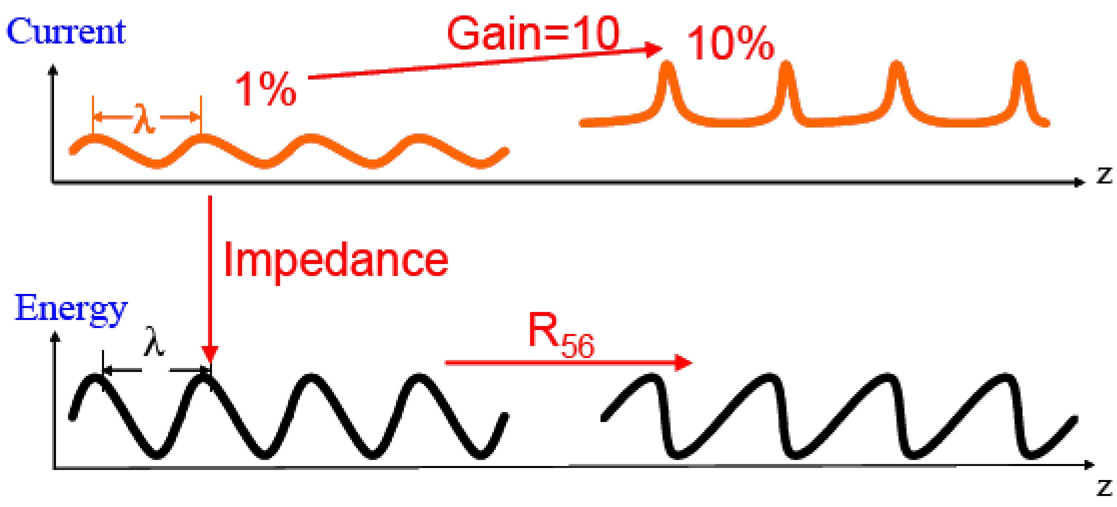
long transients



shape variation

& space charge

μ-bunch “instability”



picture from
Z. Huang, J.Wu: Microbunching instability due to bunch compression
http://icfa-usa.jlab.org/archive/newsletter/icfa_bd_nl_38.pdf

impedances (steady state):

$$Z_{\mathrm{SC}} \propto i\frac{k}{\gamma^2}\ln\left(\frac{\gamma}{k\sigma_r}\right)$$

“SC-instability”

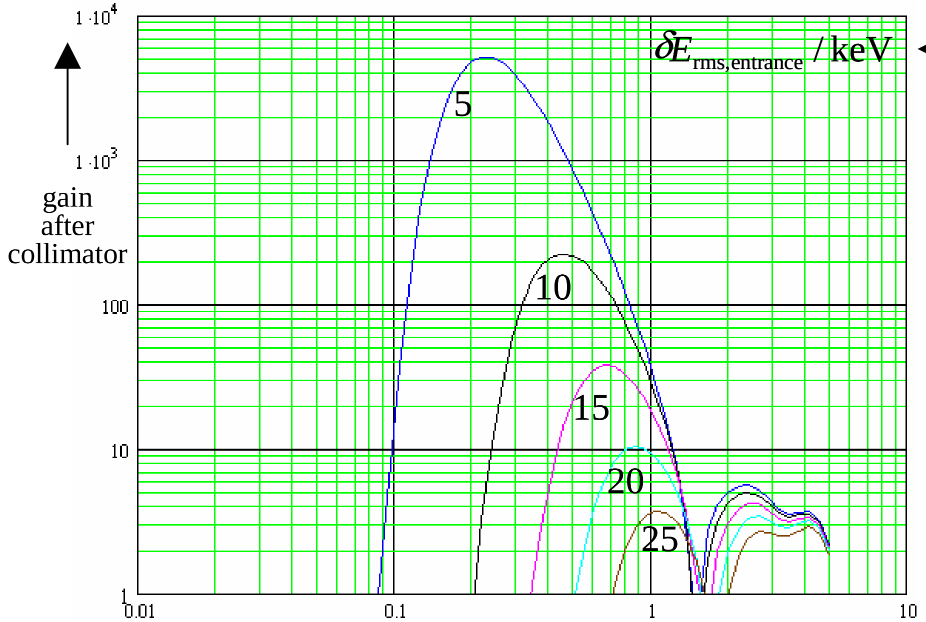
(free space, $k\sigma_r/\gamma \ll 1$)

$$Z_{\mathrm{CSR}} \propto \sqrt[3]{\frac{k}{3iR_{curv}^2}}$$

“CSR-instability”

gain curves of μ-bunch “instability”

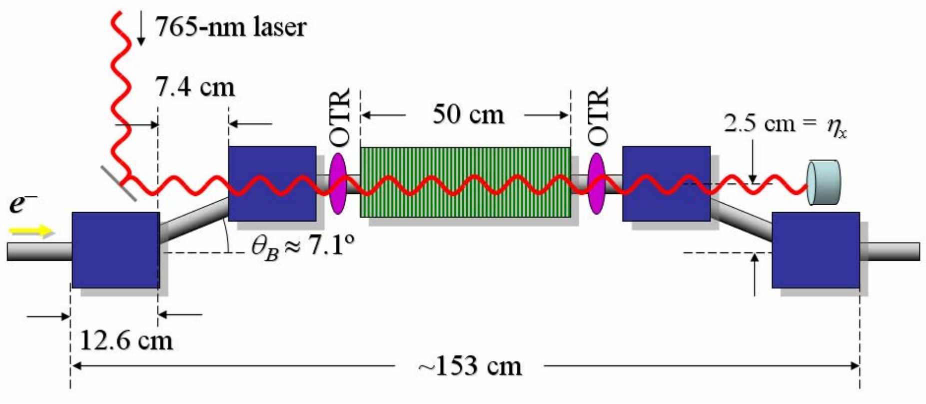
overall gain for different uncorrelated
energy spreads



wavelength before bc1 / mm

increase uncorrelated energy spread
by laser heater

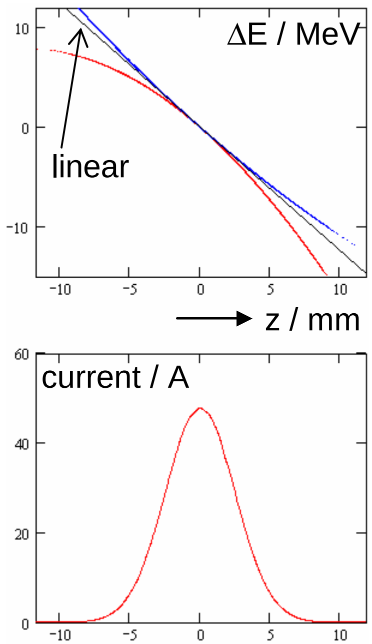
‘laser heater’ System
(LCLS layout)



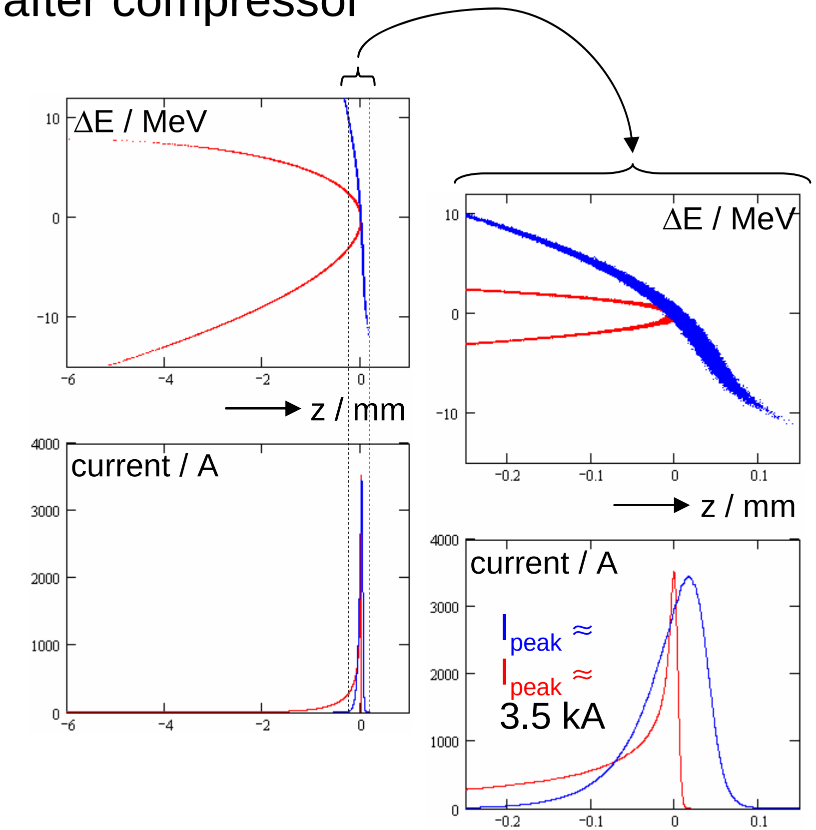
non linear effects in long. phase space

‘controlled’ or linearized compression (LCLS, European XFEL)
‘rollover’ compression (FLASH)

before compressor



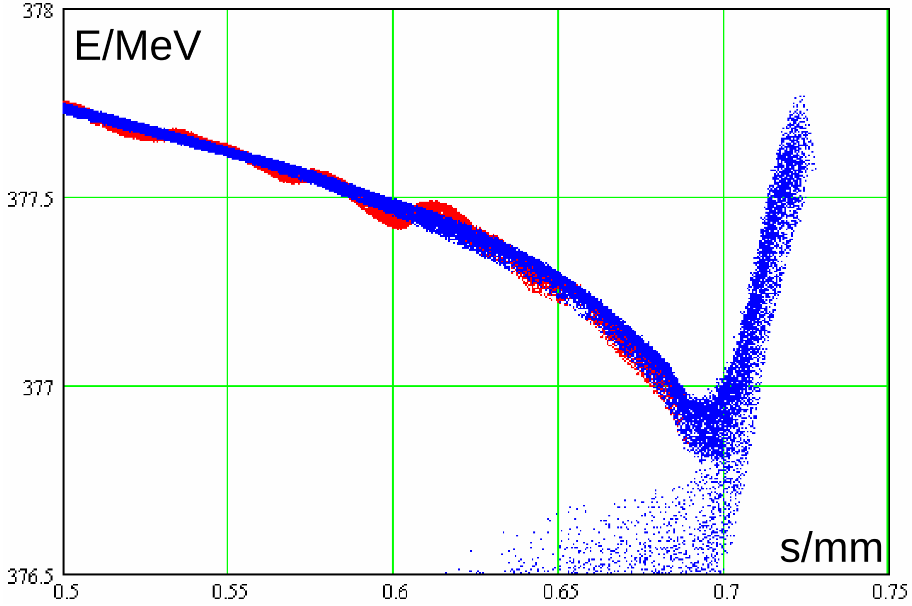
after compressor



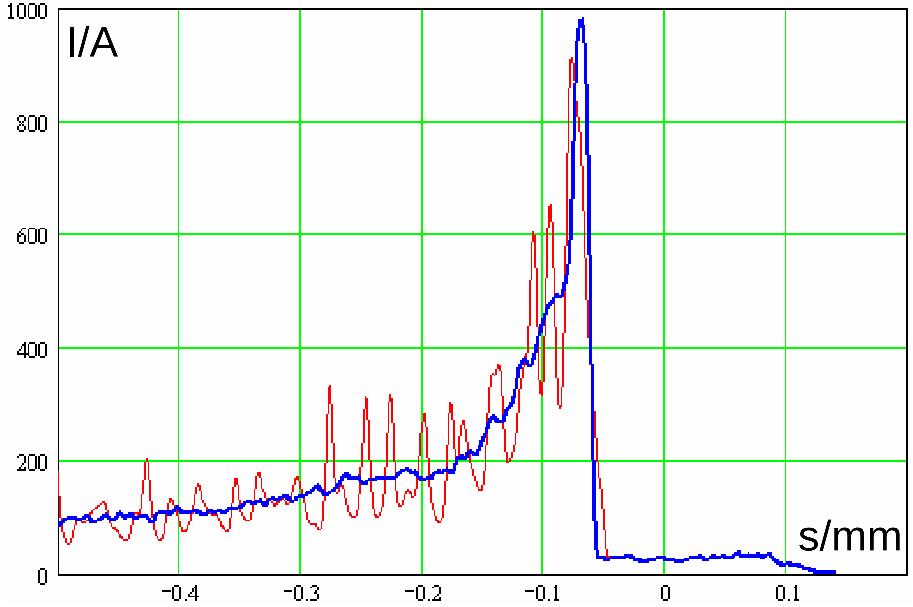
numerical noise & μ-bunch "instability"

example: rollover compression in FLASH

longitudinal phase space
before 2^{nd} BC



current after 2^{nd} BC



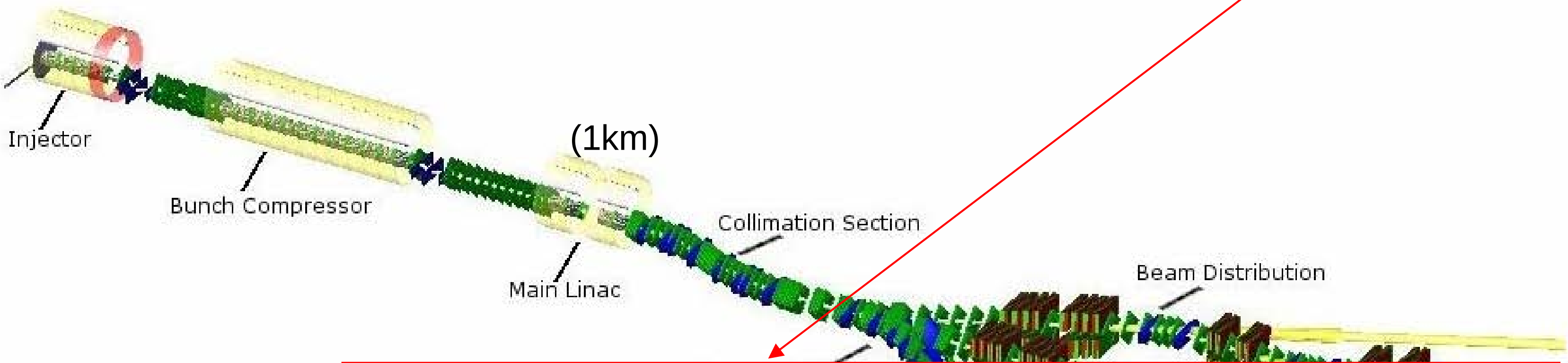
red: SC calculation with good spatial resolution
shot noise; wavelength ~ grid resolution
→ current with μ-structure
blue: reduced resolution in tail

gun to undulator tracking

Address http://www.desy.de/xfel-beam/

European XFEL Beam Dynamics Group Home Page

MAD file | **List Of Components**



1	SECTION	NAME	TYPE	LENGTH	STRENGTH	E1/LAG	E2/FREQ	TILT	S	X	Y	Z	THETA	PHI	CHI	ENERGY	BETX	ALFX	MUX	BETY	ALFY
2	[]	[]	[]	[m]	[m^(1-n)/MV]	[rad]	[rad/MHz]	[rad]	[m]	[m]	[m]	[m]	[rad]	[rad]	[rad]	[GeV]	[m]	[rad]	[2PI]	[m]	[rad]
3	INJ1	START	MARK	0.00E+00	0.00E+00	0.00000	0.000	0.000	0.000	0.00E+00	-2.75E+00	2.88E+01	0.00E+00	0.00E+00	0.00E+00	5.00E-03	3.66E+01	1.24E+01	0.00E+00	3.66E+01	1.24E
4	INJ1	GUN	MARK	0.00E+00	0.00E+00	0.00000	0.000	0.000	0.000	0.00E+00	-2.75E+00	2.88E+01	0.00E+00	0.00E+00	0.00E+00	5.00E-03	3.66E+01	1.24E+01	0.00E+00	3.66E+01	1.24E
5	ACC	START	MARK	0.00E+00	0.00E+00	0.00000	0.000	0.000	3.213	0.00E+00	-2.75E+00	3.20E+01	0.00E+00	0.00E+00	0.00E+00	5.00E-03	5.50E-01	-1.15E+00	3.73E-01	5.51E-01	-1.15E
6	ACC00	CELL1	LCAV	1.04E+00	1.05E+01	0.00000	1300.000	0.000	4.472	0.00E+00	-2.75E+00	3.33E+01	0.00E+00	0.00E+00	0.00E+00	1.55E-02	7.00E+00	-3.17E+00	4.68E-01	7.01E+00	-3.17E

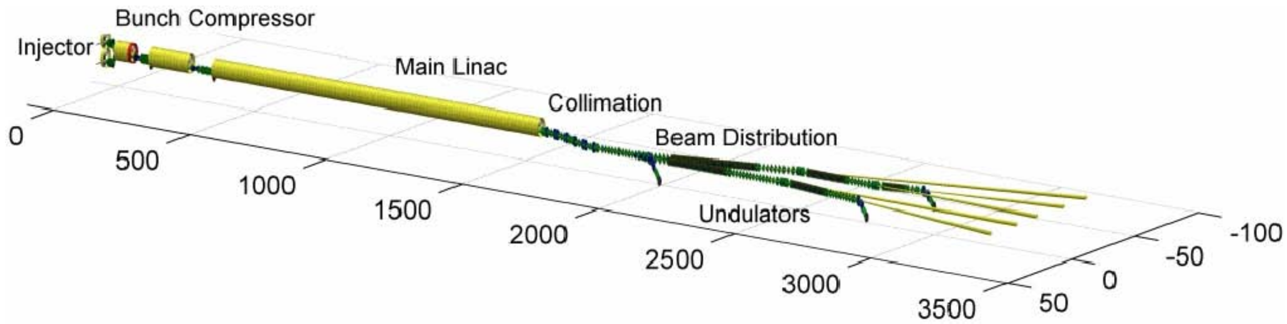
3 INJ1 START MARK . . .

1998	XS1	KVE	VKIC	2.00E-01	0.00E+00	0.00000	0.000	0.000	2142.345	0.00E+00	-2.13E+00	2.17E+03	0.00E+00	0.00E+00	0.00E+00	1.75E+01	3.64E+01	-1.92E+00	2.03E+01	2.75E+01	1.44E
1999	XS1	BPM	MONI	0.00E+00	0.00E+00	0.00000	0.000	0.000	2142.545	0.00E+00	-2.13E+00	2.17E+03	0.00E+00	0.00E+00	0.00E+00	1.75E+01	3.72E+01	-1.95E+00	2.03E+01	2.69E+01	1.41E
2000	XS1	QF.12	QUAD	5.00E-01	8.43E-02	0.00000	0.000	0.000	2143.045	0.00E+00	-2.13E+00	2.17E+03	0.00E+00	0.00E+00	0.00E+00	1.75E+01	3.76E+01	1.20E+00	2.03E+01	2.67E+01	-8.59E
2001	SASE1	START	MARK	0.00E+00	0.00E+00	0.00000	0.000	0.000	2143.045	0.00E+00	-2.13E+00	2.17E+03	0.00E+00	0.00E+00	0.00E+00	1.75E+01	3.76E+01	1.20E+00	2.03E+01	2.67E+01	-8.59E
2002	SASE1	UNDU	UNDULATO	5.00E+00	0.00E+00	0.00000	0.000	0.000	2148.045	0.00E+00	-2.13E+00	2.18E+03	0.00E+00	0.00E+00	0.00E+00	1.75E+01	2.72E+01	8.78E-01	2.03E+01	3.69E+01	-1.18E
2003	SASE1	BS	RBEN	2.15E-01	0.00E+00	0.00000	0.000	0.000	2148.420	0.00E+00	-2.13E+00	2.18E+03	0.00E+00	0.00E+00	0.00E+00	1.75E+01	2.65E+01	8.54E-01	2.03E+01	3.78E+01	-1.21E

2002 SASE1 UNDU UNDULATO . . .

2488	DUMP2	BV.1	RBEN	5.00E+00	-8.73E-02	0.00000	0.000	-1.571	3059.050	-1.13E+01	-3.94E+00	3.09E+03	-1.75E-01	2.30E-02	-7.10E-17	1.75E+01	4.23E+02	-1.85E+01	2.74E+01	2.51E+02	-2.94E
2489	DUMP2	QG.2	QUAD	3.00E+00	-7.76E-01	0.00000	0.000	0.000	3063.050	-1.14E+01	-4.63E+00	3.09E+03	-1.75E-01	2.30E-02	-7.10E-17	1.75E+01	3.09E+03	-1.45E+03	2.74E+01	1.96E+01	3.95E
2490	DUMP2	BPM	MONI	0.00E+00	0.00E+00	0.00000	0.000	0.000	3063.050	-1.14E+01	-4.63E+00	3.09E+03	-1.75E-01	2.30E-02	-7.10E-17	1.75E+01	3.09E+03	-1.45E+03	2.74E+01	1.96E+01	3.95E
2491	DUMP2	QG.3	QUAD	3.00E+00	7.63E-01	0.00000	0.000	0.000	3067.050	-1.15E+01	-5.33E+00	3.10E+03	-1.75E-01	2.30E-02	-7.10E-17	1.75E+01	3.17E+03	2.23E+03	2.74E+01	2.39E+03	-1.28E
2492	DUMP2	BPM	MONI	0.00E+00	0.00E+00	0.00000	0.000	0.000	3067.050	-1.15E+01	-5.33E+00	3.10E+03	-1.75E-01	2.30E-02	-7.10E-17	1.75E+01	3.17E+03	2.23E+03	2.74E+01	2.39E+03	-1.28E
2493	DUMP2	SWEEP	KICK	5.00E-01	0.00E+00	0.00000	0.000	0.000	3068.550	-1.16E+01	-5.59E+00	3.10E+03	-1.75E-01	2.30E-02	-7.10E-17	1.75E+01	9.71E+00	-1.24E+02	2.79E+01	7.75E+03	-2.30E
2494	DUMP2	DUMP	DUMP	1.00E+00	0.00E+00	0.00000	0.000	0.000	3077.550	-1.18E+01	-7.15E+00	3.11E+03	-1.75E-01	2.30E-02	-7.10E-17	1.75E+01	1.29E+05	-1.43E+04	2.79E+01	1.04E+05	-8.43E

European XFEL, segmentation



130 MeV			500 MeV			2 GeV
gun	acc0 + …	dogleg	heater & linac 1	bc1	linac 2	bc2
cathode cavity solenoid	module quad	dipoles quads	modules (1st & 3rd) quads	dipoles	modules quads	dipoles

17.5 GeV				
main linac	colli-mator	…	SASE1	…
modules quads	dipoles quads		undulator (with quads)	

rf, dispersion

gun to undulator tracking : technical aspects

rf settings: phase and amplitude settings are very sensitive
wakes & space charge effects change longitudinal profile significantly!
$\rightarrow$ iterative optimization

matching: real
artificial

steering

bunch: 1nC, ~50A (initial)

simulation: s2e particles (ASTRA-generator & gun simulation)
$N_{s2e} \approx 200000$
try to track these particles; avoid conversions to other distributions (if possible);

utility programs

format conversion: ASTRA / CSRtrack / sdds

some simple manipulations of longitudinal phase space:

add cavity wakes (based on point particle wakes,
asymptotic fit to ECHO calculations),

add space charge wakes (semi analytic model)

some simple manipulations of transverse phase space:
(transport matrices)

drift,

transport as defined by linear optics (design),

matching

codes

some available tracking programs

Astra, Parmela, GPT: space charge effects $\rightarrow$ Poisson solver
external fields (magnets, cavities)

Trafic^4, CSRtrack: space charge and CSR effects;
PEC shielding (planar chamber);
external fields (magnets)

Elegant: external fields (magnets, cavities) & wakes
simple 1d CSR model

some more:
MAFIA, ITACA, SPIEFE, TREDI, ATRAP, HOMDYN
single particle:
AT, BETA, BMAD, COMFORT, COSY-INFINITY, DIMAD, LEGO, LIAR, LUCRETIA, MAD, MARYLIE, MERLIN, ORBIT, PETROS, PLACET, PTC, RACETRACK, SAD, SIXTRACK, SYNCH, TEAPOT, TRACY, TRANSPORT, TURTLE, UAL **(from W. Decking)**
more: CHEF, ILCv, LUCRETIA, MATLIAR, SLEPT, …

FEL codes

FAST
Genesis
Ginger (2d)

some more:
3d: FELEX, FELOS, RON,
FELS, FRED3D, MEDUSA, TDA3D
2d: NUTMEG
1d: FS1T, SARAH
(from S. Reiche)

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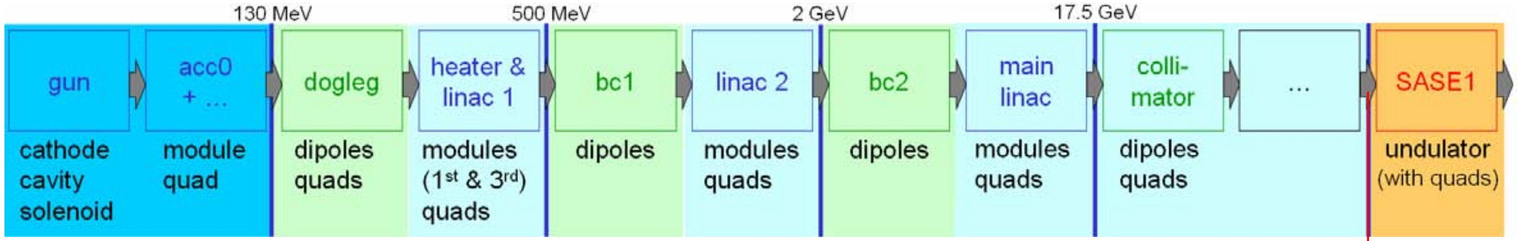
parallel versions available for most codes
time consuming: CSR effects by sub-bunch method
SASE-FEL

computational effort

example: European XFEL

method 1 (fast)

ASTRA | CSRtrack 1d | transport matrix | GENESIS | rf-field cavity wake & s.c. field



8 h | 20 min | 30 min | 30 min | sec…min (steady state)

PC (Pentium 4, 3GHz)

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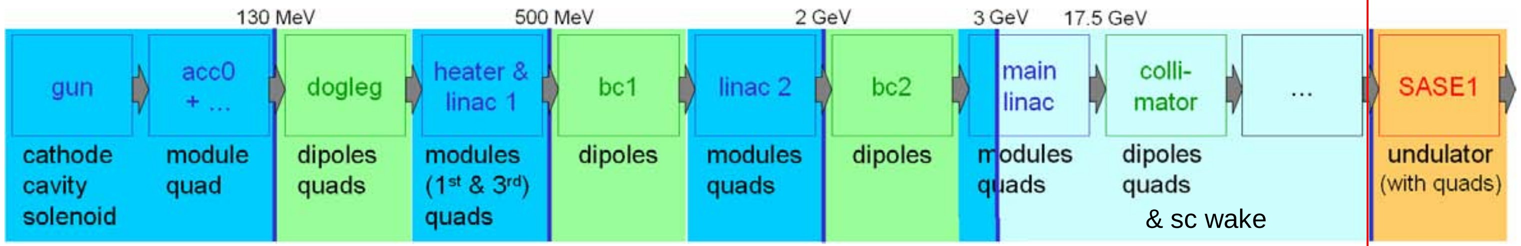
method 2 (reference)

ASTRA | CSRtrack sub-bunch | ELEGANT | GENESIS

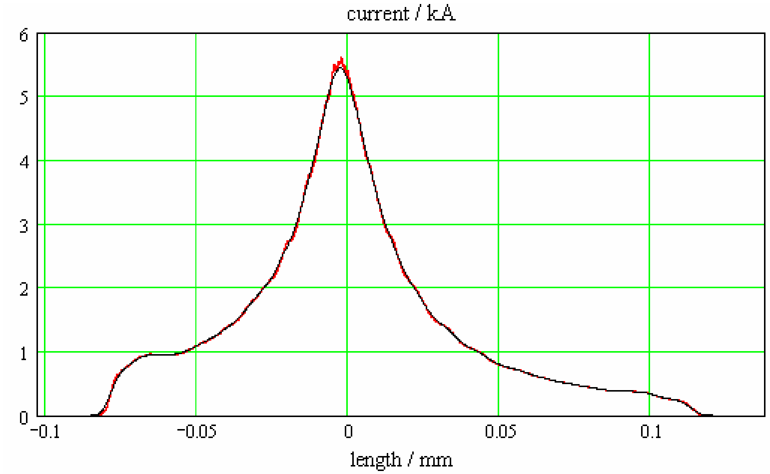


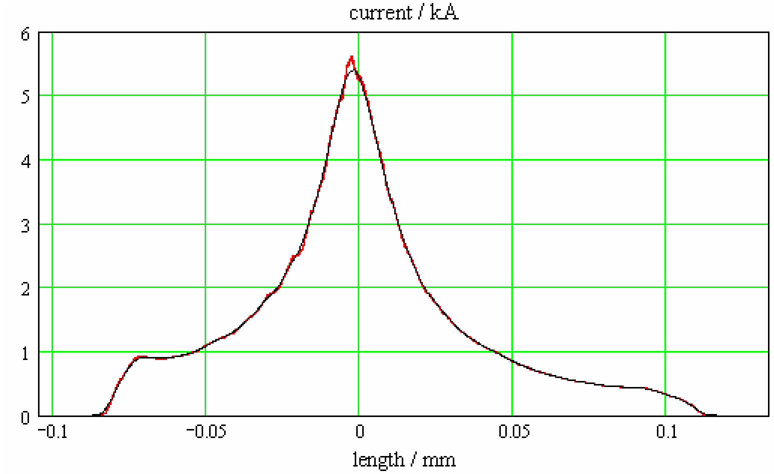
1.5 h | 2 h | 30 h | 4 h | 12 h | 3 h | h…w (SASE)

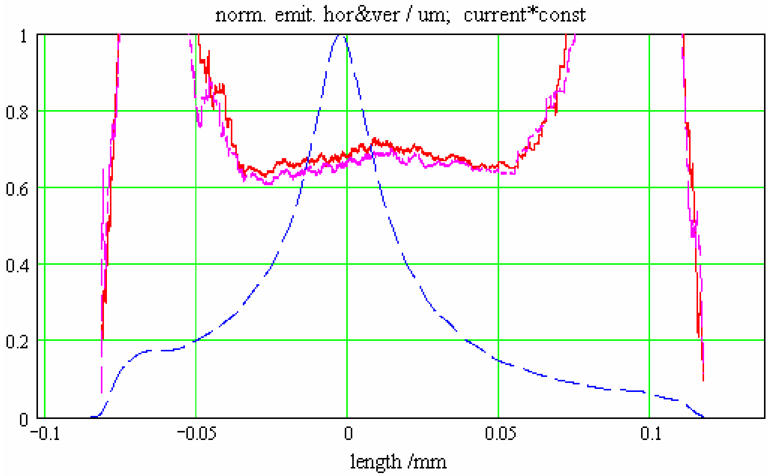
LINUX cluster with 20 cpus (64 bit)

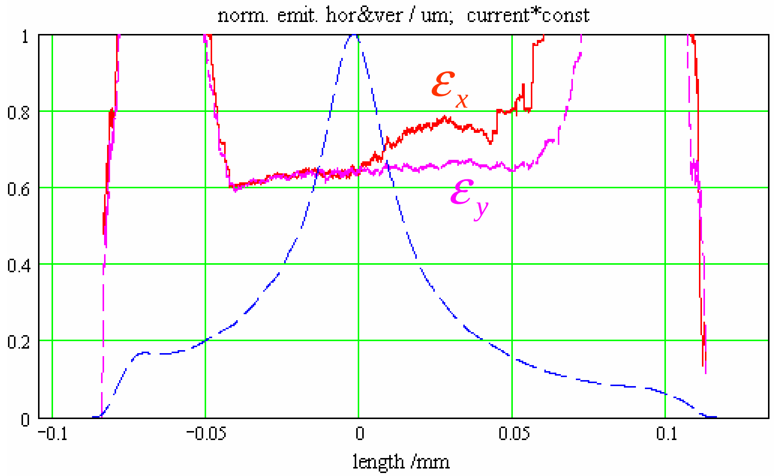
method 1	method 2

current & slice emittance



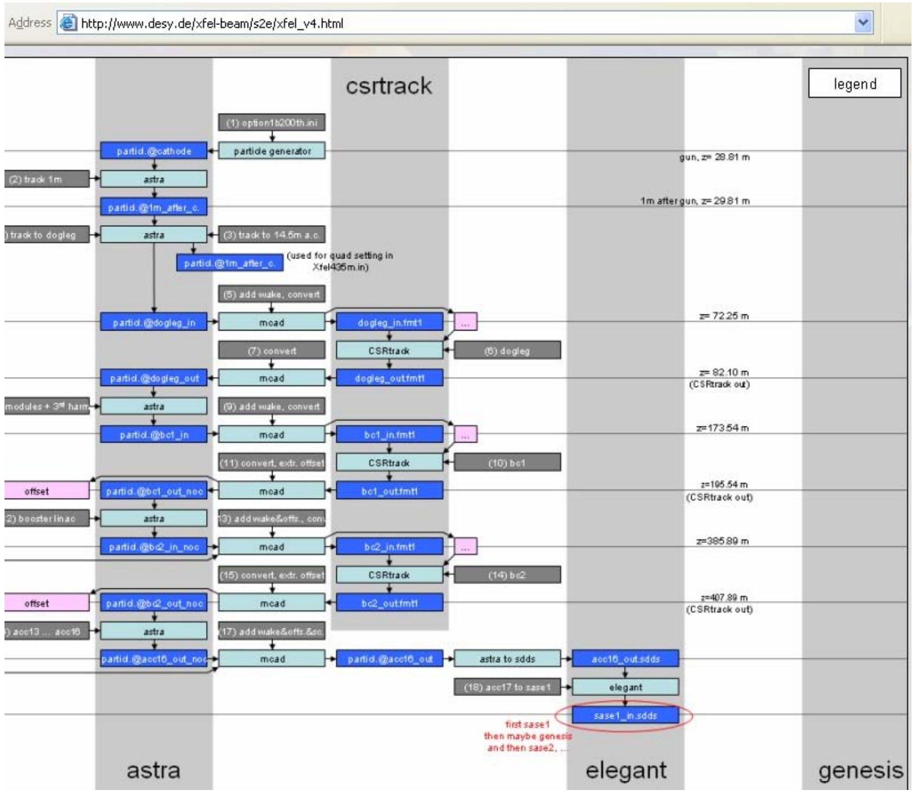






s2u: {many codes & glue} $\leftrightarrow$ s2e-code

European XFEL



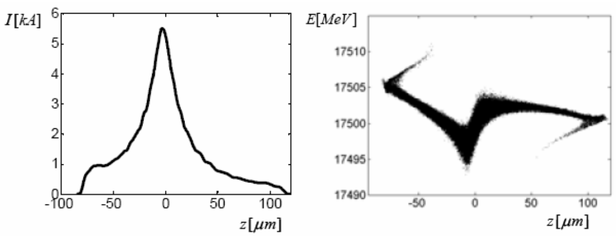
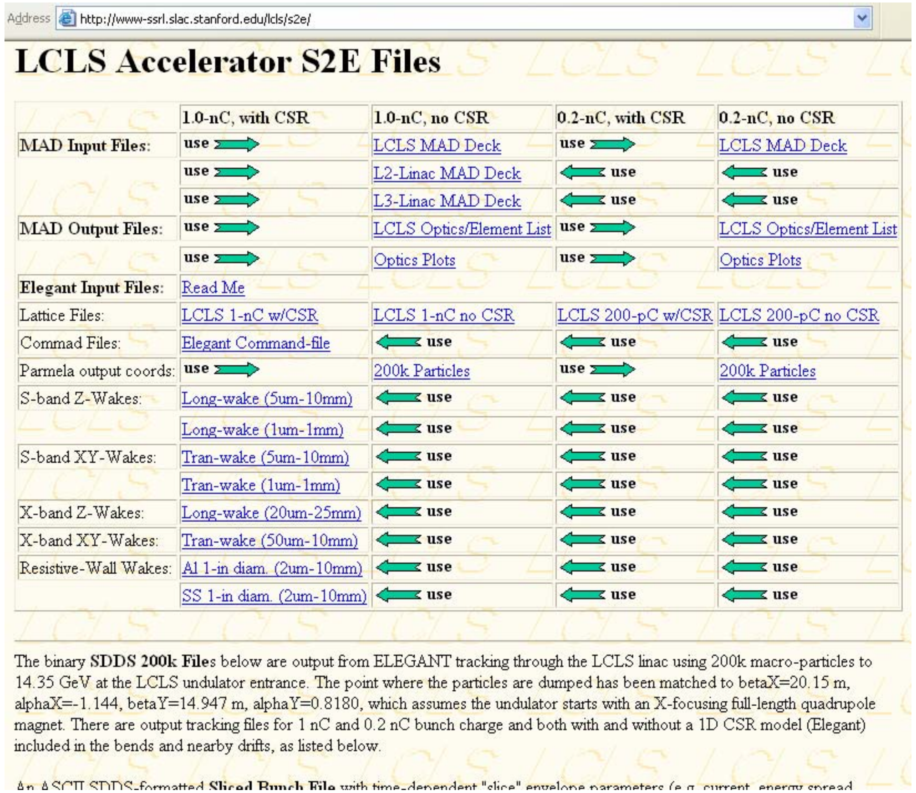


Figure 1: Current profile and longitudinal phase space at the undulator entrance (1nC at 17.5GeV)

LCLS



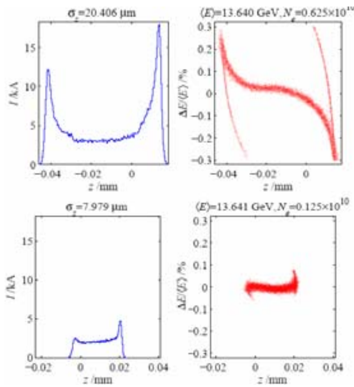
Address http://www-ssrl.slac.stanford.edu/lcls/s2e/

LCLS Accelerator S2E Files

	1.0-nC, with CSR	1.0-nC, no CSR	0.2-nC, with CSR	0.2-nC, no CSR
MAD Input Files:	use →	LCLS MAD Deck	use →	LCLS MAD Deck
	use →	L2-Linac MAD Deck	← use	← use
	use →	L3-Linac MAD Deck	← use	← use
MAD Output Files:	use →	LCLS Optics/Element List	use →	LCLS Optics/Element List
	use →	Optics Plots	use →	Optics Plots
Elegant Input Files:	Read Me			
Lattice Files:	LCLS 1-nC w/CSR	LCLS 1-nC no CSR	LCLS 200-pC w/CSR	LCLS 200-pC no CSR
Commad Files:	Elegant Command-file	← use	← use	← use
Parmela output coords:	use →	200k Particles	use →	200k Particles
S-band Z-Wakes:	Long-wake (5um-10mm)	← use	← use	← use
	Long-wake (1um-1mm)	← use	← use	← use
S-band XY-Wakes:	Tran-wake (5um-10mm)	← use	← use	← use
	Tran-wake (1um-1mm)	← use	← use	← use
X-band Z-Wakes:	Long-wake (20um-25mm)	← use	← use	← use
X-band XY-Wakes:	Tran-wake (50um-10mm)	← use	← use	← use
Resistive-Wall Wakes:	Al 1-in diam. (2um-10mm)	← use	← use	← use
	SS 1-in diam. (2um-10mm)	← use	← use	← use

The binary **SDDS 200k Files** below are output from ELEGANT tracking through the LCLS linac using 200k macro-particles to 14.35 GeV at the LCLS undulator entrance. The point where the particles are dumped has been matched to betaX=20.15 m, alphaX=-1.144, betaY=14.947 m, alphaY=0.8180, which assumes the undulator starts with an X-focusing full-length quadrupole magnet. There are output tracking files for 1 nC and 0.2 nC bunch charge and both with and without a 1D CSR model (Elegant) included in the bends and nearby drifts, as listed below.

Longitudinal phase space in FEL at 13.6 GeV with 1-nC (top) and 0.2-nC (bottom). Plots show the longitudinal distribution (left), and phase space. Bunch head at $z < 0$.



FEL & SASE: usual approximations

particle motion and wave-particle interaction
are averaged over one or more wiggler wavelength

$$\frac{\partial \gamma}{\partial z} = -\frac{e}{mc^2}\left\langle \frac{\mathbf{E}\cdot\mathbf{v}}{v} \right\rangle$$

resonant approximation

$$k_l = 2\pi/\lambda_l$$

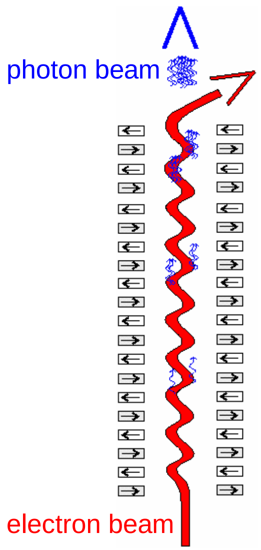
$$\mathbf{E} \approx \mathrm{Re}\left\{\underbrace{\tilde{\mathbf{E}}_\perp(\mathbf{r},t)}_{\text{slowly in } z \text{ and } t}\exp\left(i\, k_l (z - t/c)\right)\right\} + E_z \mathbf{e}_z$$

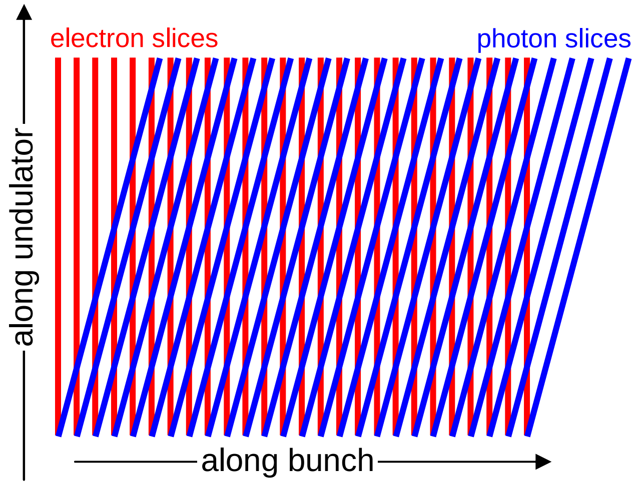
paraxial approximation

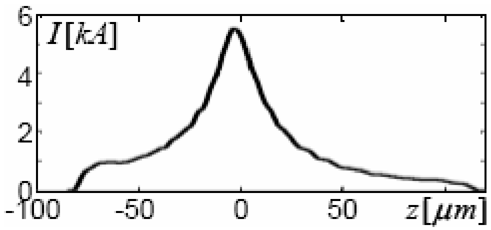
$$\left(\nabla_\perp^2 + 2ik\left(\frac{\partial}{\partial z} + \frac{1}{c}\frac{\partial}{\partial t}\right)\right)\tilde{\mathbf{E}}_\perp = -i\mu_0\omega\tilde{\mathbf{J}}_\perp$$

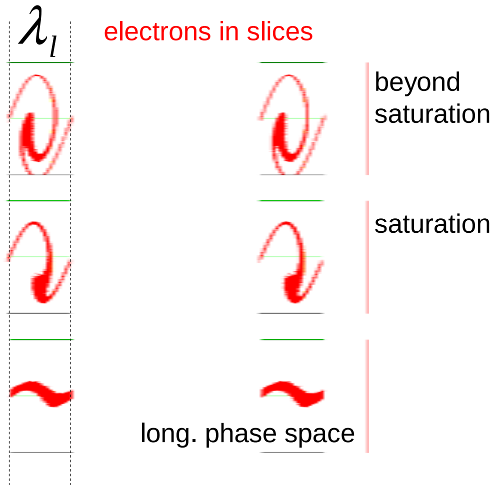
SASE: macro particles with controlled shot noise

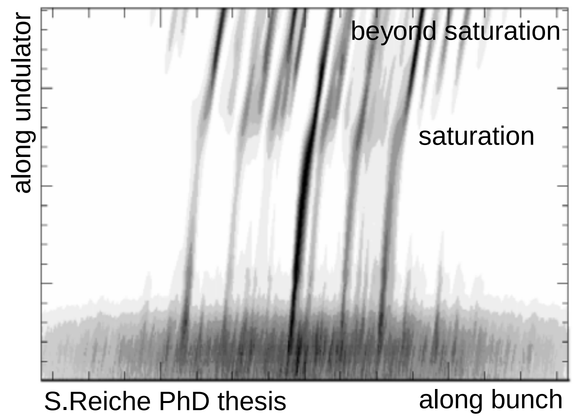
SASE simulation











example: European XFEL, 1nC, 0.1nm

length along undulator = 135 m

step along undulator: $4\lambda_u$ particles per slice ~ 10000

step along bunch: $64\lambda_l$ number of slices ~ 10000

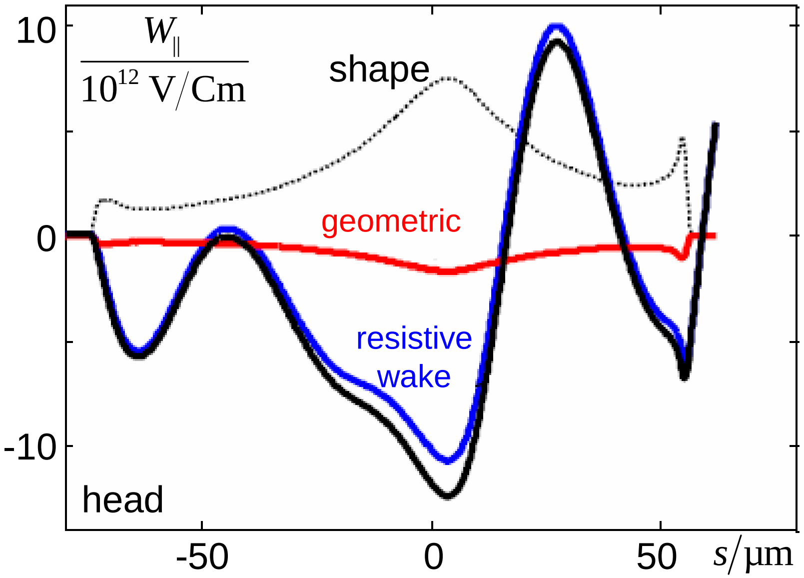
90 min / seed 150 seeds $\rightarrow$ ~ 10 days

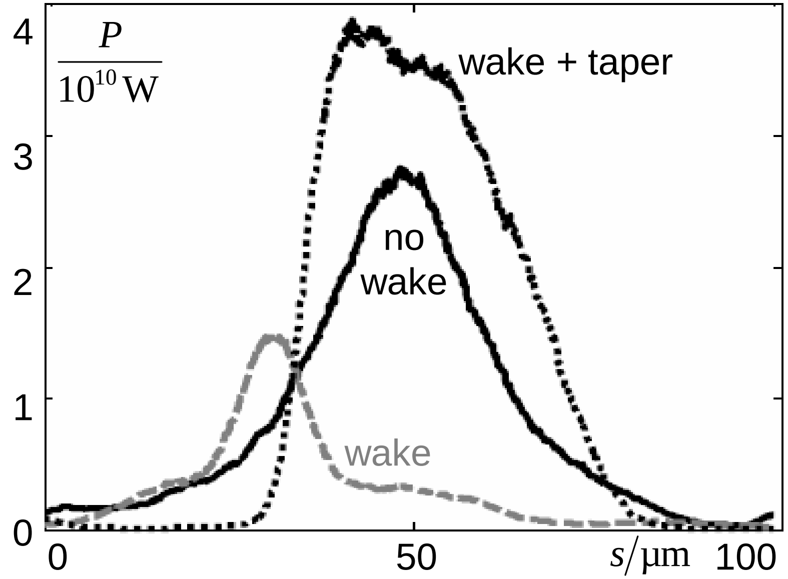
LINUX cluster with 20 cpus (64 bit)

undulator-to-end simulation

Igor Zagorodnov

bunch shape and
different contributions
to long. wake in undulator



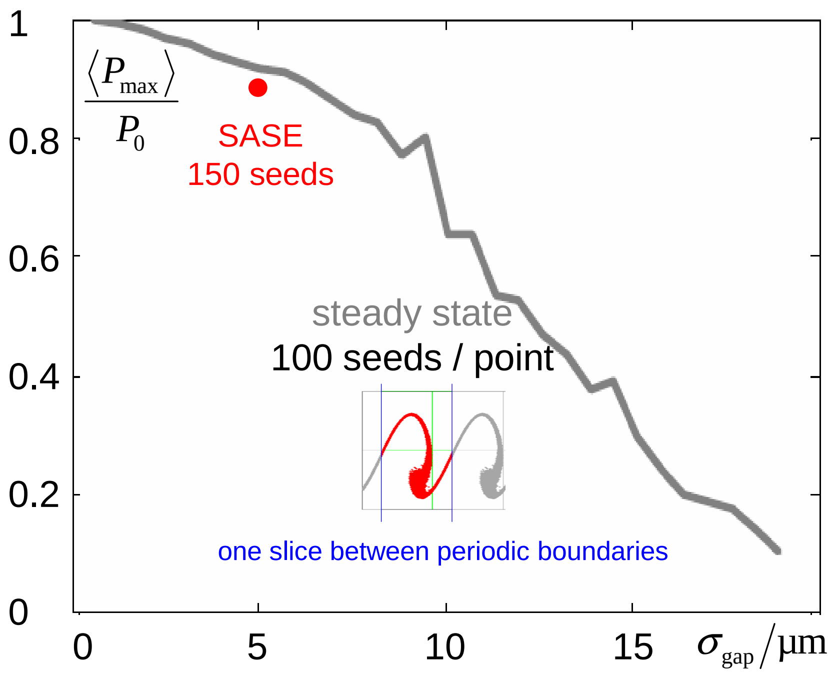


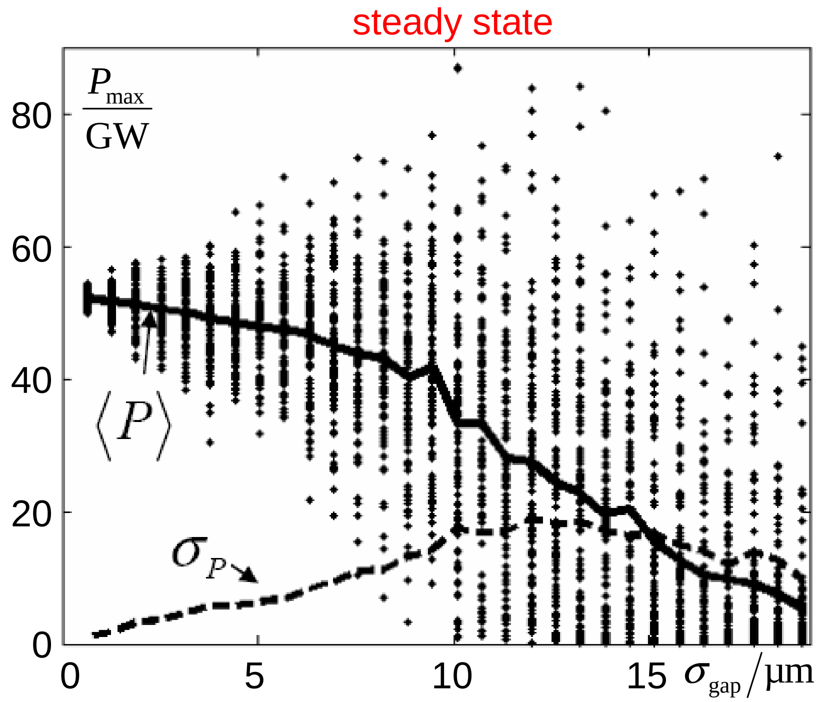
$$\lambda_l = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2}\right)$$

the energy loss along the undulator
can be compensated by tapering

a tolerance study

(impact of undulator gap)





SASE model ~ 10000 slices

steady state model: one slice between periodic boundaries

example: European XFEL, 1nC, 0.1nm

steady state 30 sec / seed 100 seeds / $\rightarrow$ ~ 1 h all points $\rightarrow$ ~ 1 day

SASE 90 min / seed 150 seeds $\rightarrow$ ~ 10 days

PC (Pentium 4, 3GHz), LINUX cluster with 20 cpus (64 bit)

summary

complicated beam dynamics even before undulator

emittance compensation in gun, longitudinal compression,
sensitive longitudinal dynamic, importance of wakes, SC & CSR effects,
unwanted μ-bunching before undulator

fast approaches for particular effects

e.g. parameter sensitivity, μ-bunch instability, steady state

gun to undulator tracking

input from other investigations (wakes)
few CSR codes, fewer available, non with all possibilities (e.g. resistive wakes)
parallel SC & CSR programs
use of different methods and codes (SC, CSR)
interfaces: change of format / phase space description
careful control of parameters (real settings / computational)
"glued" multi method computations have been done
(but need experience and careful inspection of intermediate results)

SASE-FEL

input from other investigations (surface properties, wakes)
efficient "steady state" computations, SASE is time consuming (needs parallel c.)
SASE-FEL codes need experience (many parameters)