Computational Needs for the XFEL

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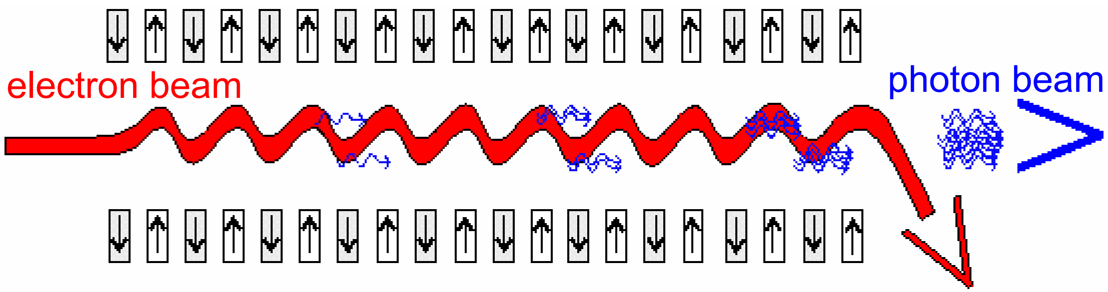
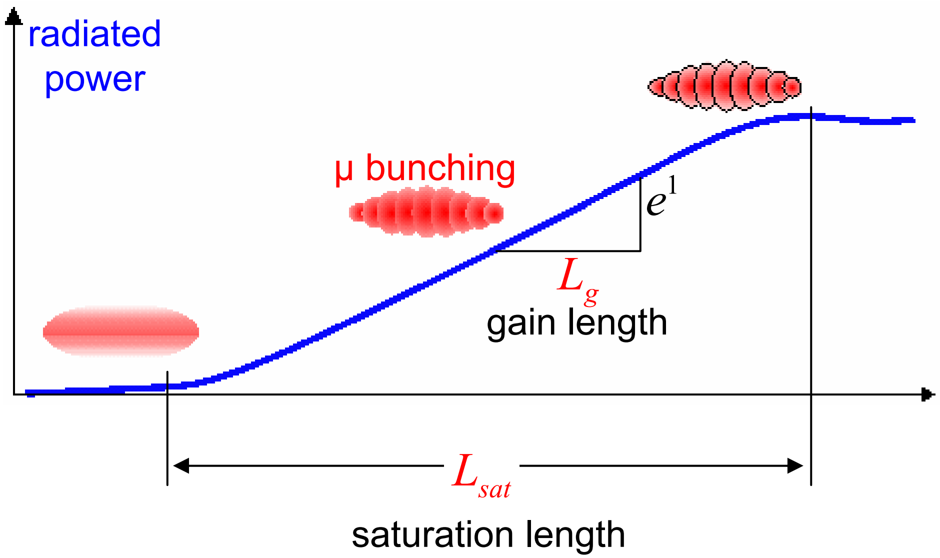
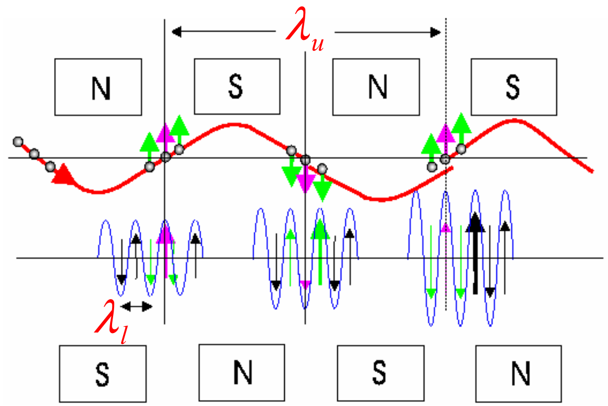
TOC

about FELs: SASE XFEL





resonant interaction:



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

what are the physical challenges?

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

$K \propto 1$

$\lambda_u \propto \text{cm}$

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

FLASH 13nm@690MeV

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

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

$L_u > L_{sat} \propto 10 L_g$

$\propto 100\ \text{m}$

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

$$L_g \propto \left[\frac{2mc}{\mu_0 e}\frac{\gamma^3\lambda_u}{K^2}\frac{\sigma_r^2}{\hat{I}}\right]^{1/3}$$

(1d FEL theory)

$L_u > L_{sat} \propto 10\,L_g$

current density

$\hat{I} \approx 1 \cdots 10\,\text{kA}$

FLASH ~ 100μm
LCLS, E-XFEL ~ 30μm

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

overlap of photon & electron beam

emittance $\varepsilon \propto < \lambda_l$

normalized emittance $\varepsilon_n \approx 1\ \mu\text{m}$

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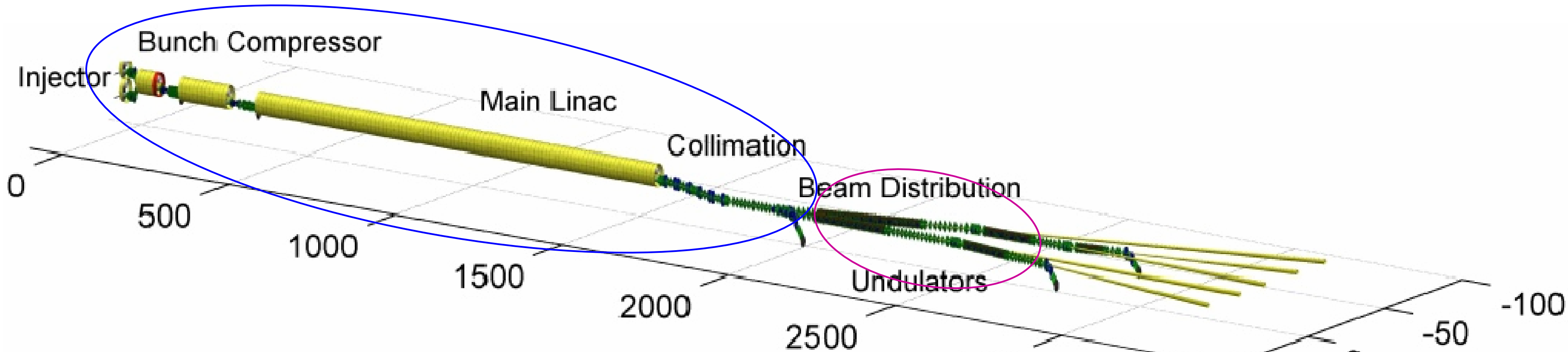
energy spread ↔ bandwidth $\Delta E / E \propto \lambda_u / L_g \propto 10^{-4}$

accelerator and SASE FEL



beam preparation

- gun
- injector
- BC system
- linac

FEL & SASE

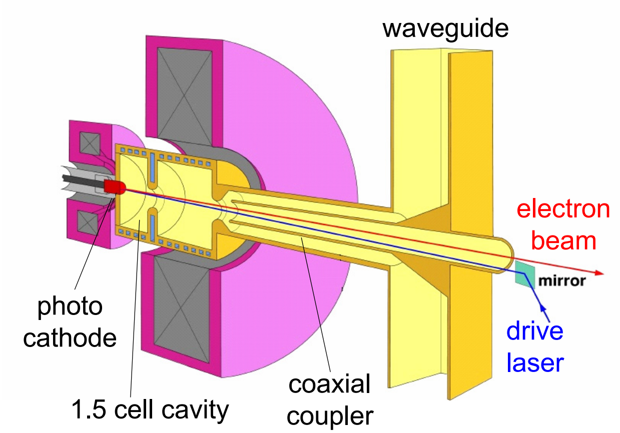
source: jitter & fluctuations
driven fields: field errors, alignment
self fields: space charge, CSR, wakes

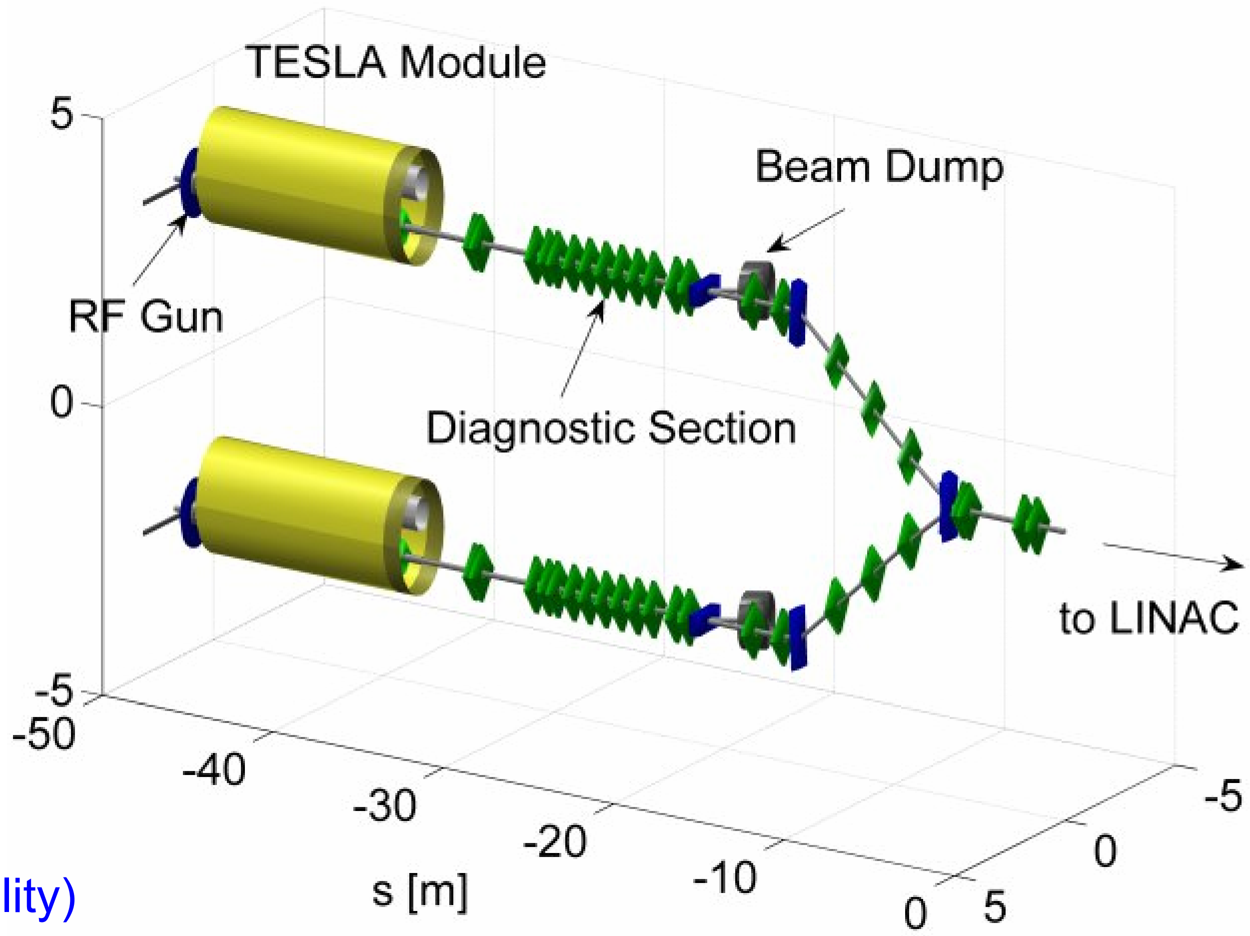
parameter sensitivity, μ-bunch (in)stability, undulator orbit

gun & injector

~ 10 … 100 A; ~ 100 MeV

RF Gun





drive laser
external fields (field stability)
space charge effects

bunch compression system

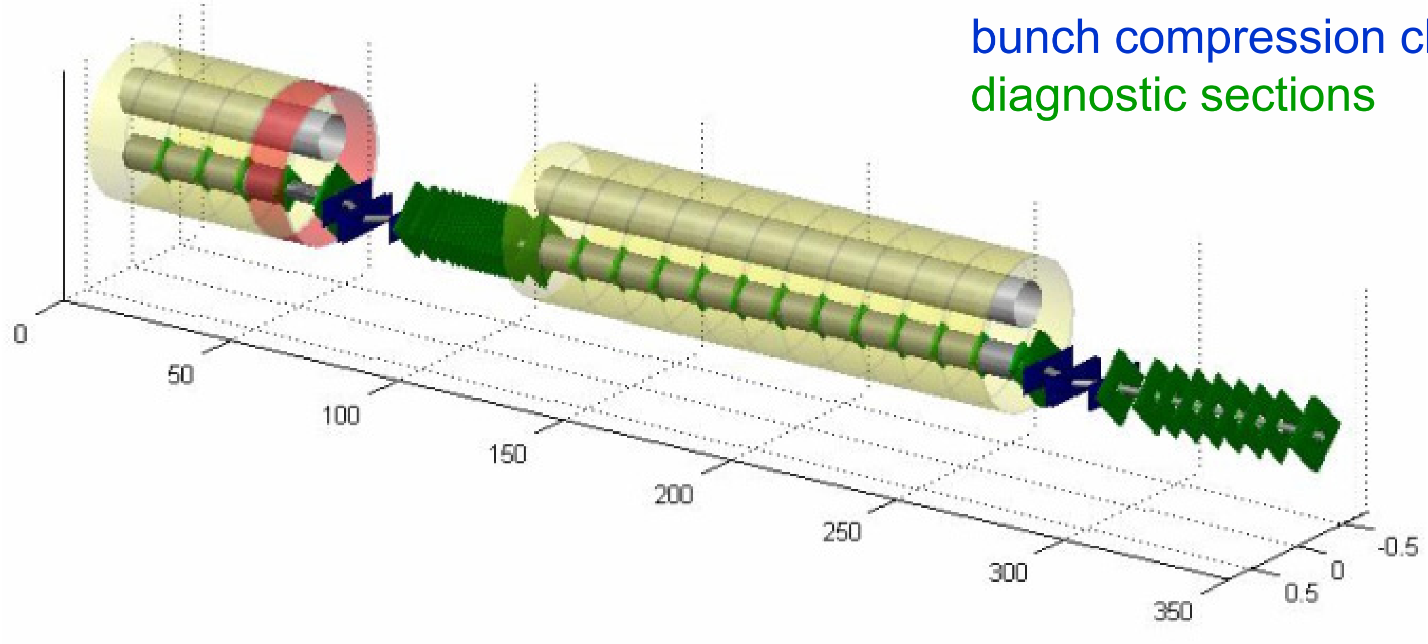
→ 1 … 10 kA; → ~ 20 GeV

1.3 GHz rf

3.9 GHz rf (linearization)

bunch compression chicanes

diagnostic sections



external fields (field stability)

space charge effects

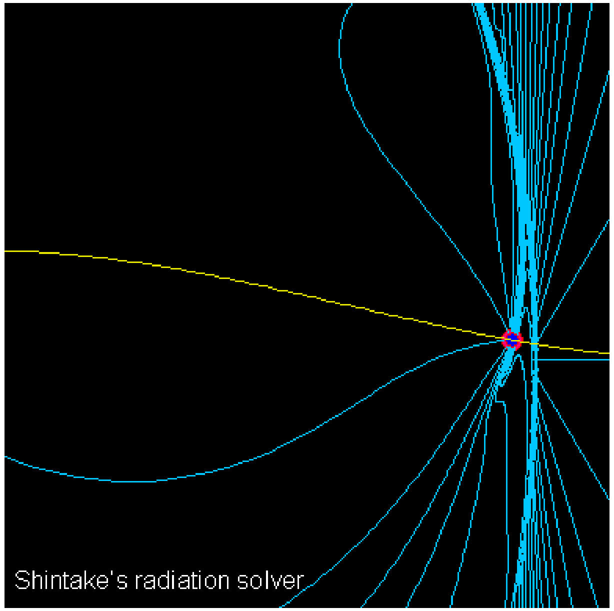
coherent synchrotron radiation

wakes {dispersion free solvers, general indirect wake integrators}

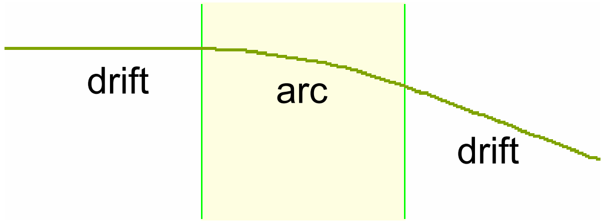
CSR effects

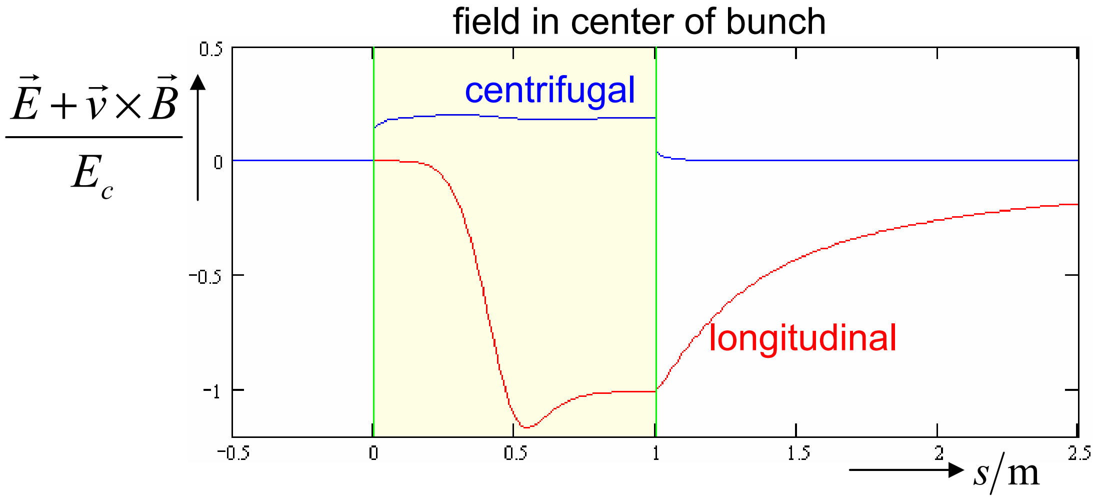
radiation effects

overtaking



long transients:

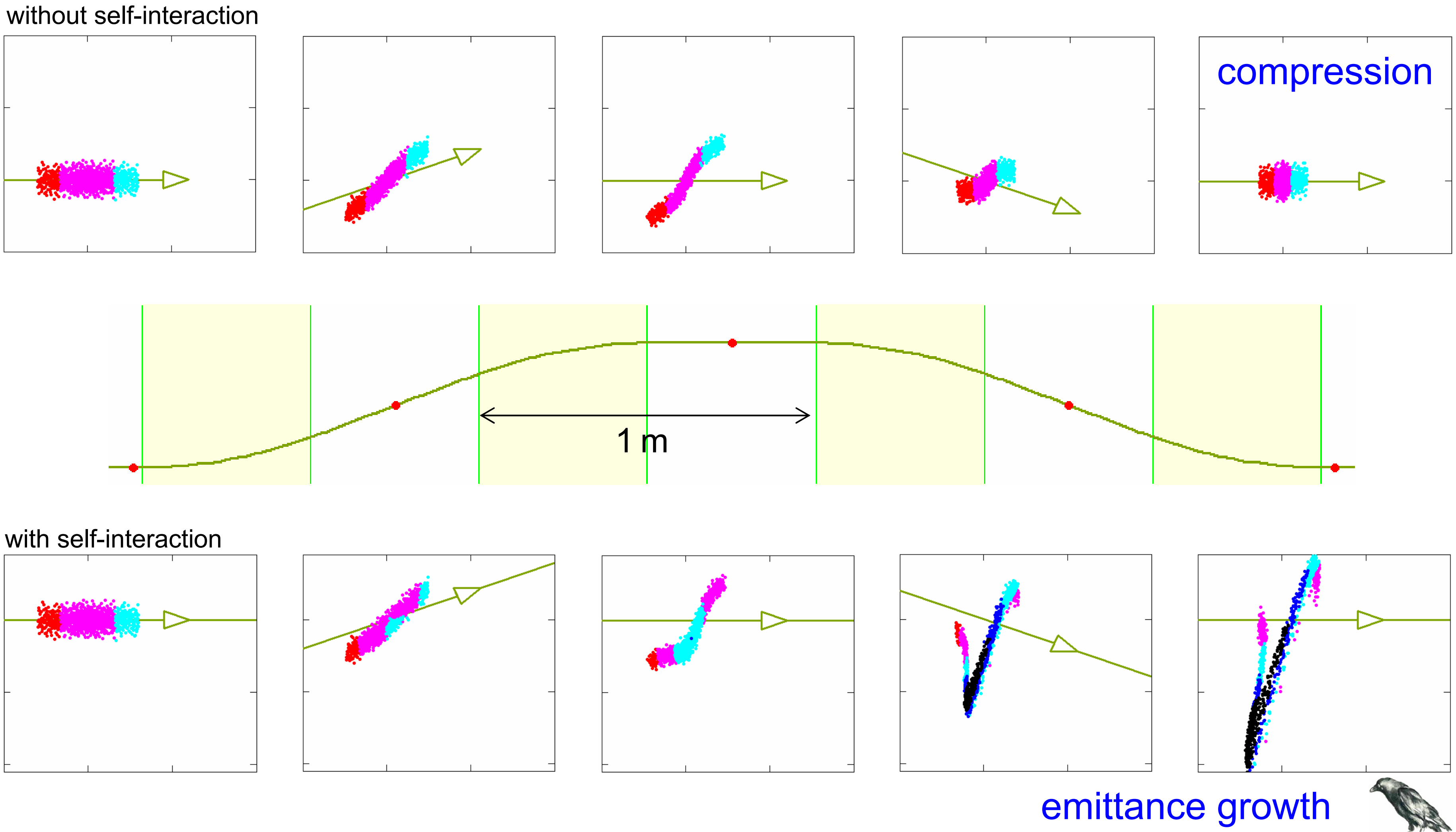




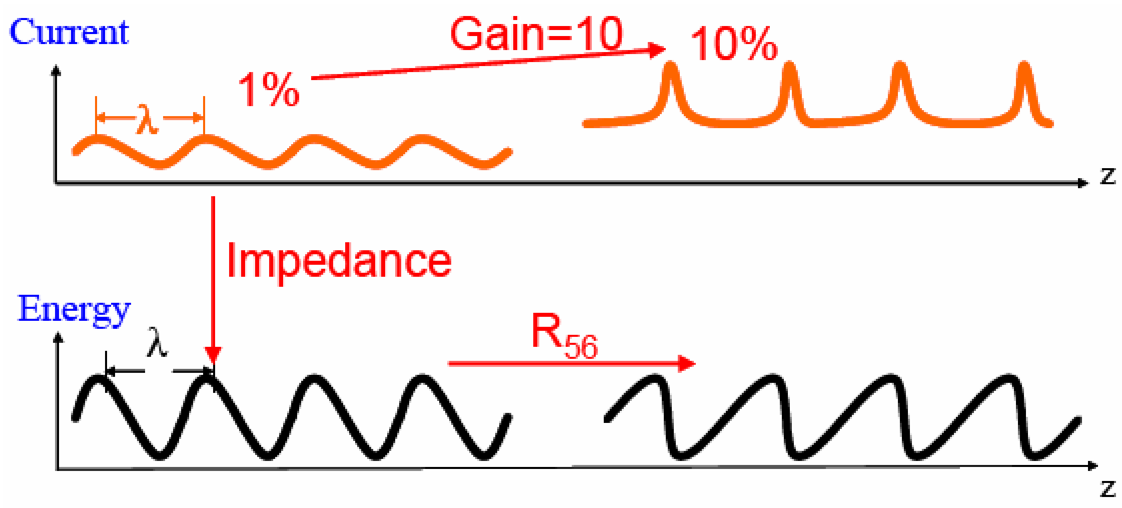
… CSR effects

shape variation

top view (horizontal plane), color = energy



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):

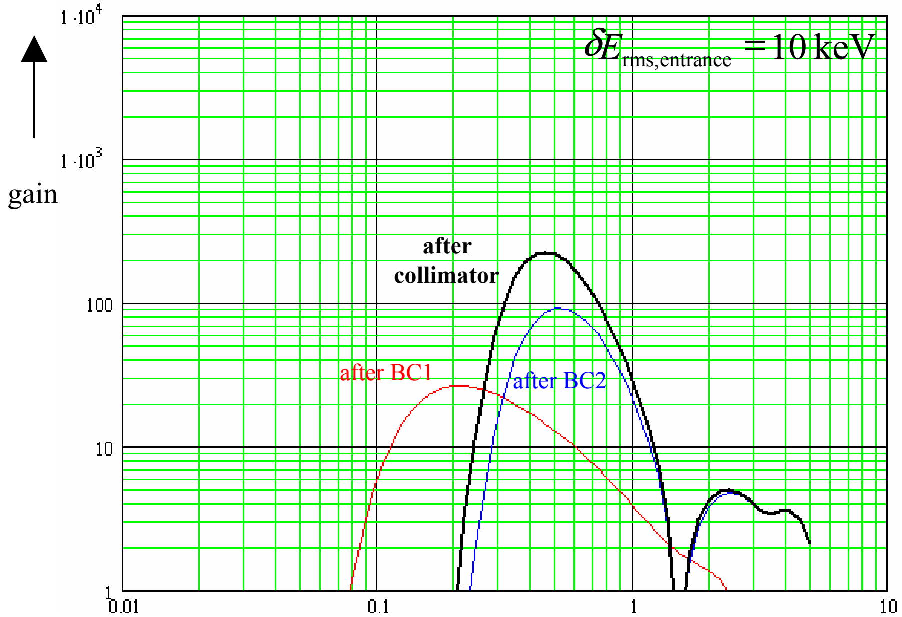
$$Z_{\mathrm{SC}} \propto i\frac{k}{\gamma^2}\ln\left(\frac{\gamma}{k\sigma_r}\right)$$ “SC-instability”

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

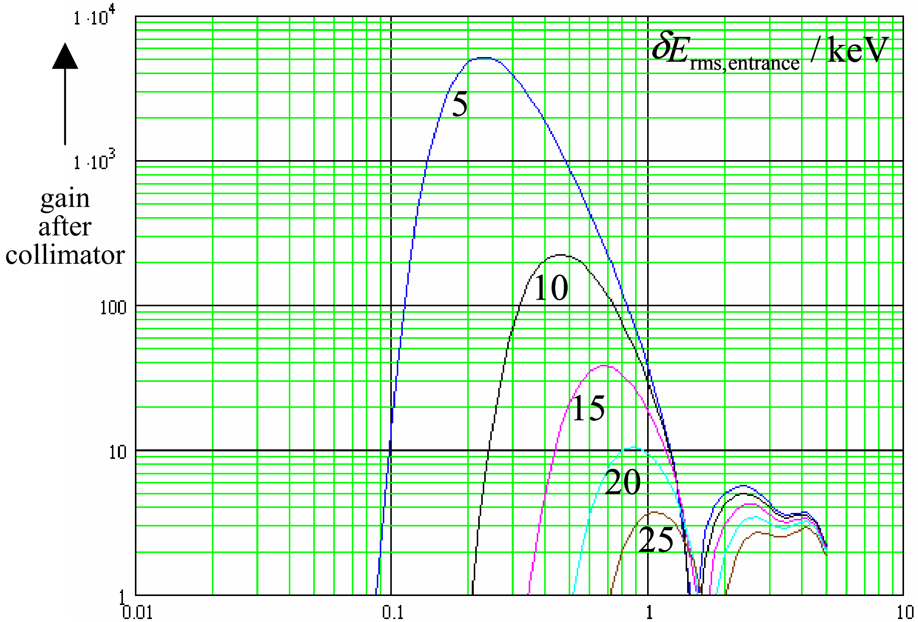
$$Z_{\mathrm{CSR}} \propto \sqrt[3]{\frac{k}{3iR_{curv}^2}}$$ “CSR-instability”

gain curves of µ-bunch "instability"

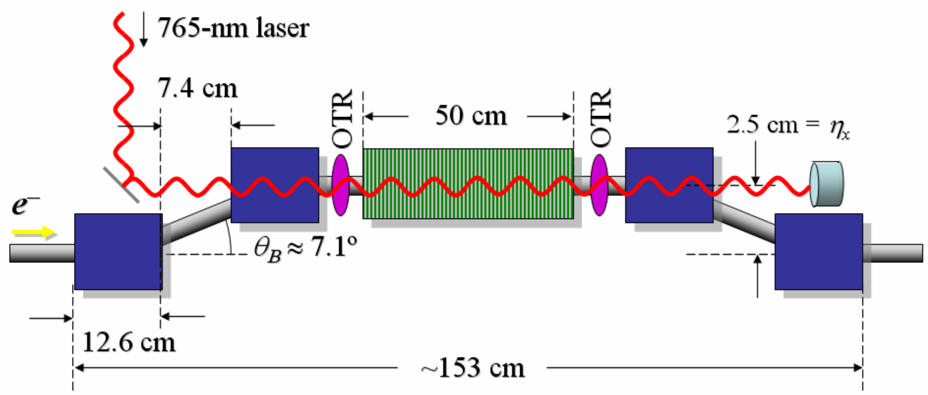
contributions of the sub-sections of the linac for an uncorrelated energy spread of 10 keV



overall gain for different uncorrelated energy spreads



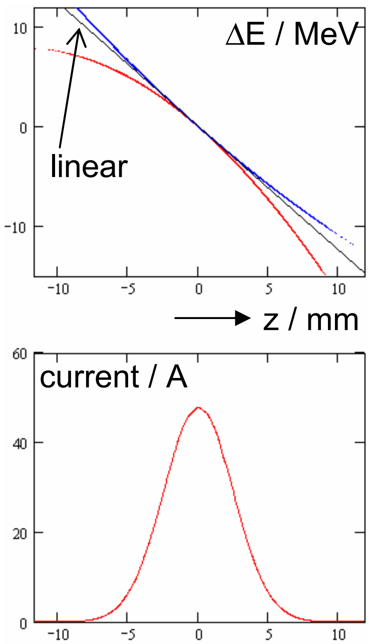
'laser heater' System (LCLS layout)



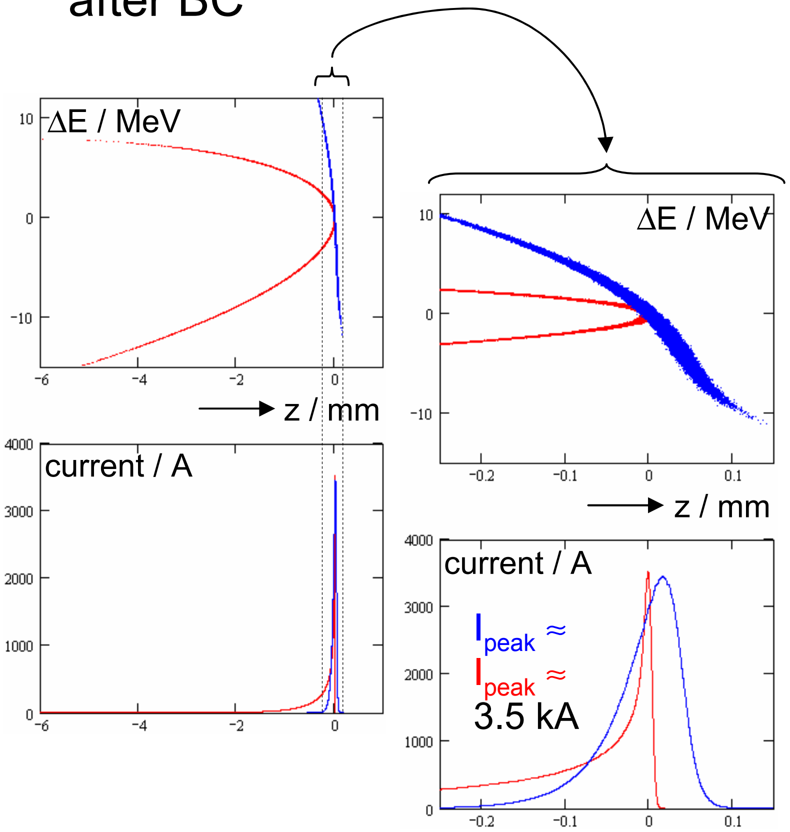
non linear effects in long. phase space

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

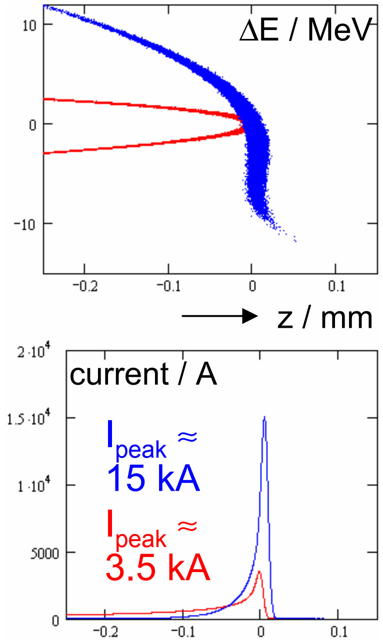
before BC



after BC



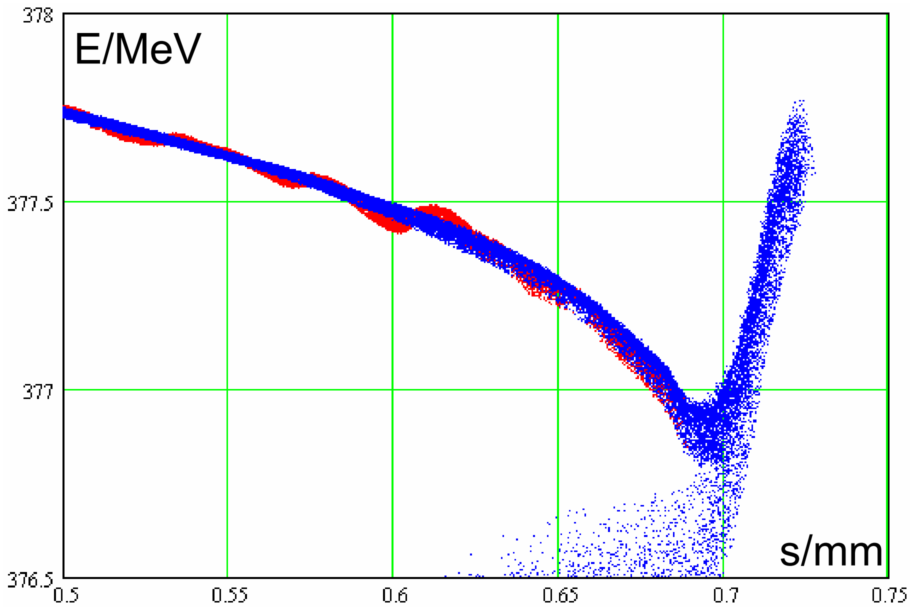
lost control:
magnet strength changed by 0.5%



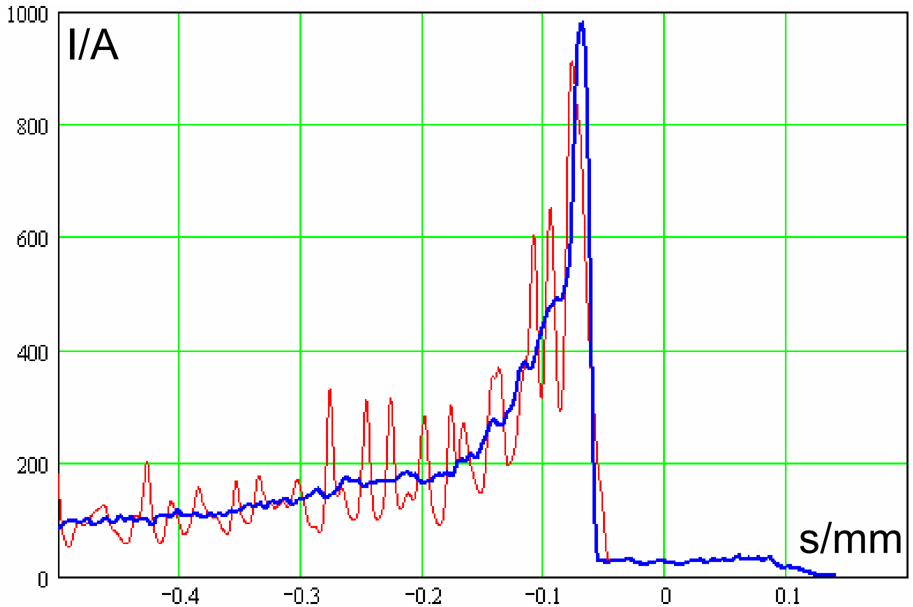
numerical noise & μ-bunch “instability”

example: rollover compression in FLASH

longitudinal phase space
before 2^{nd} BC



current after 2^{nd} BC



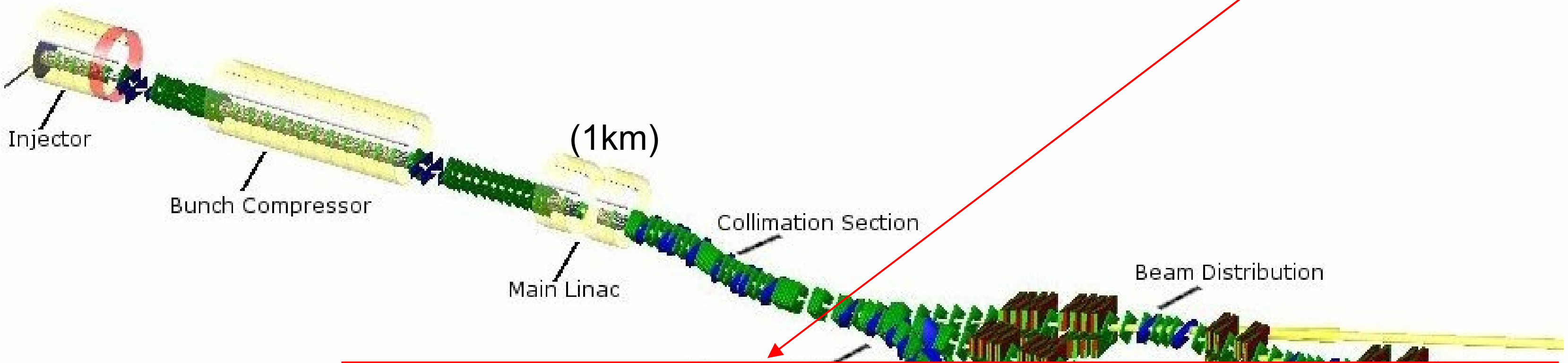
red: SC calculation with good spatial resolution
shot noise; wavelength ~ grid resolution
→ current with μ-structure
blue: reduced resolution in tail

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

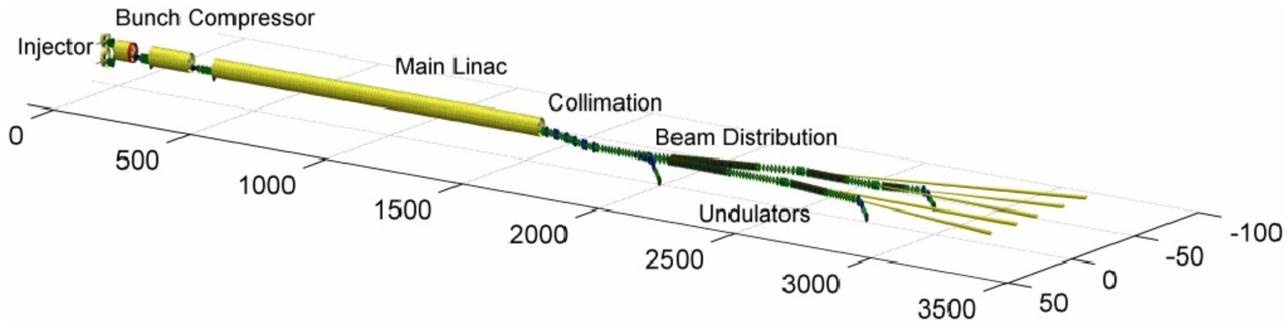
3	INJ1	START	MARK	. . .

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



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

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

rf, dispersion

codes

some available tracking programs

Astra, Parmela, GPT: space charge effects → 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)**

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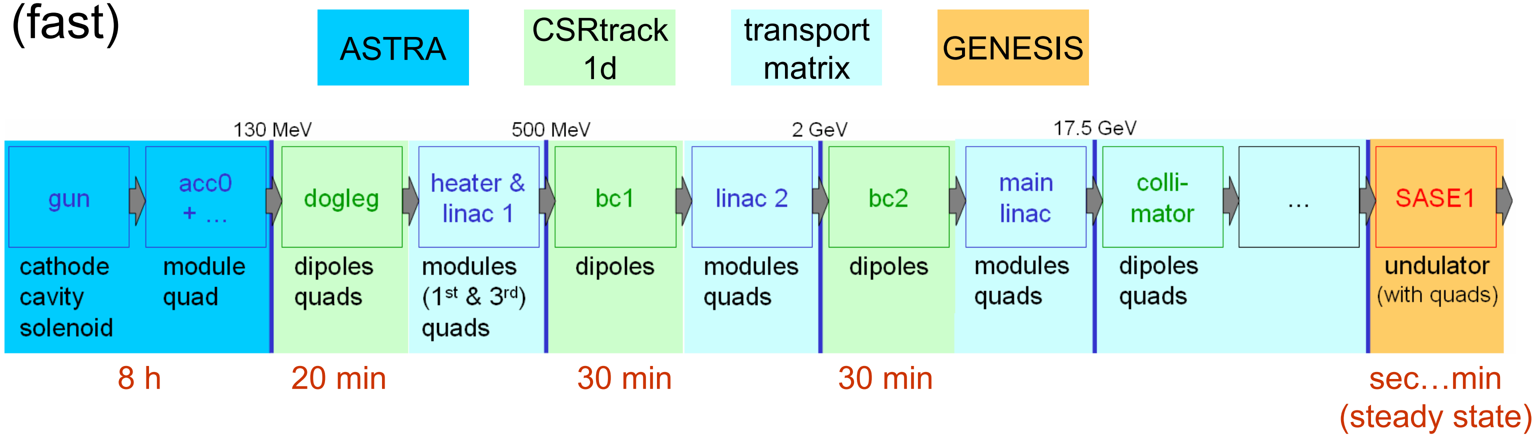
parallel versions available for most codes
time consuming: CSR effects by sub-bunch method
SASE-FEL

computational effort

example: European XFEL

method 1 (fast)



PC (32 bit)

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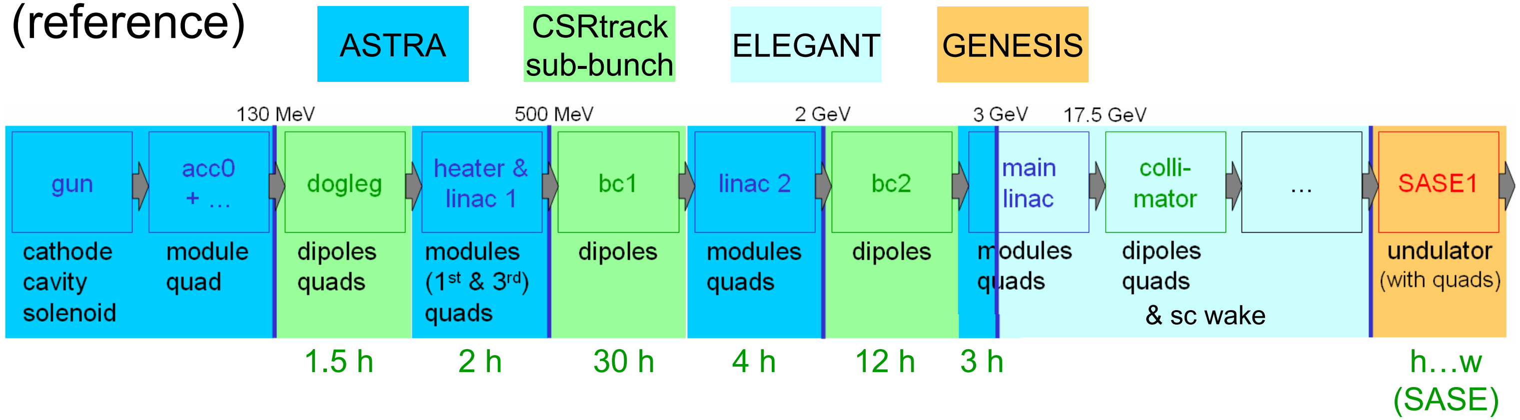
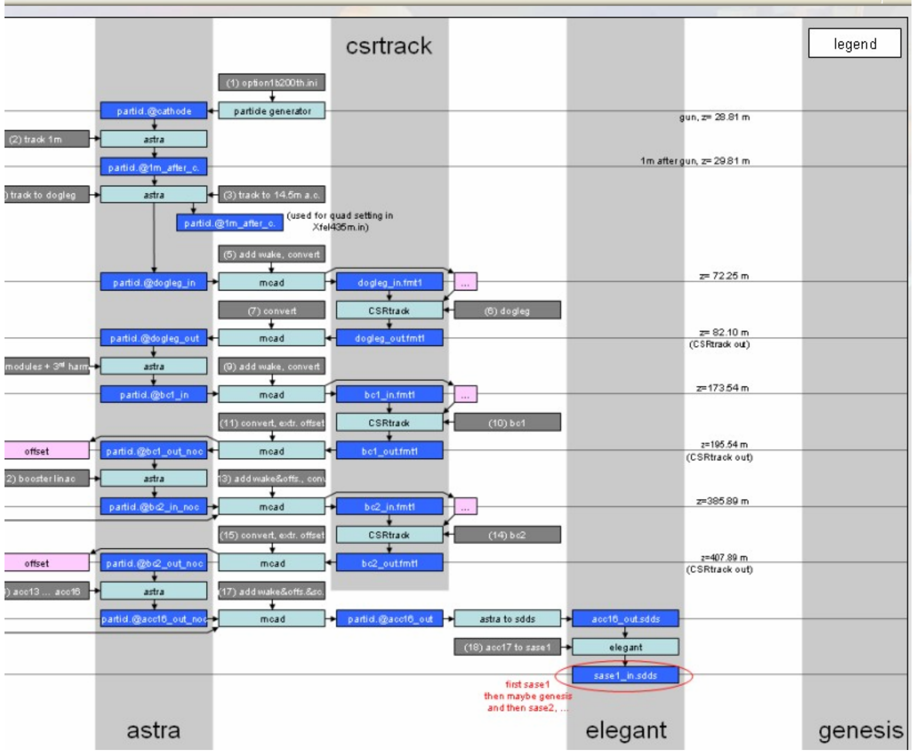
method 2 (reference)



LINUX cluster with 20 cpus (64 bit)

s2u: {many codes & glue} ↔ s2e-code

European XFEL



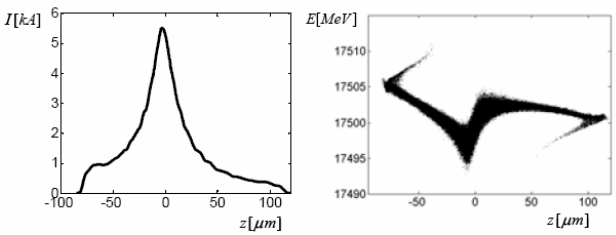


Figure 1: Current profile and longitudinal phase space at the undulator entrance (1nC at 17.5GeV)

LCLS

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

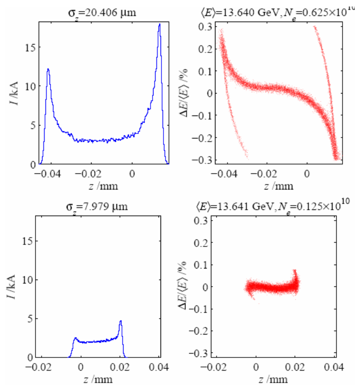
LCLS Accelerator S2E Files

	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.

An ASCII SDDS-formatted **Sliced Bunch File** with time-dependent "slice" envelope parameters (e.g. σ, current, energy spread

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

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

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

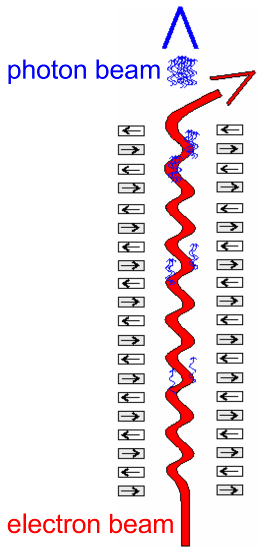
slowly in z and t

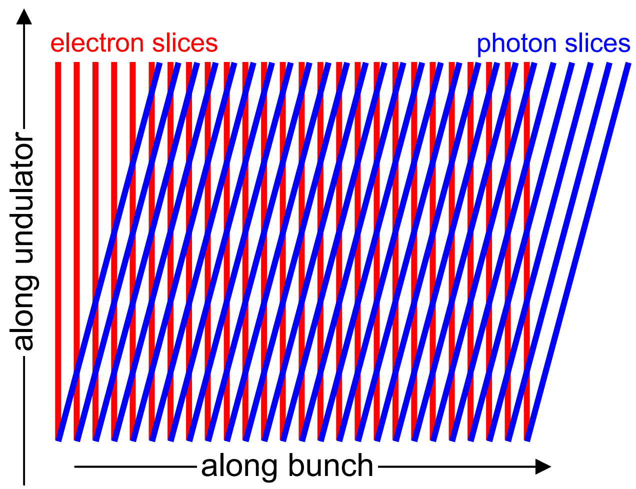
paraxial approximation

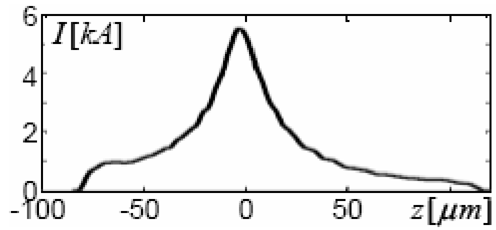
$$\left(\nabla_\perp^2 + 2ik\left(\frac{\partial}{\partial z} + \frac{1}{c}\frac{\partial}{\partial t}\right)\right)\widetilde{\mathbf{E}}_\perp = -i\mu_0 \omega \widetilde{\mathbf{J}}_\perp$$

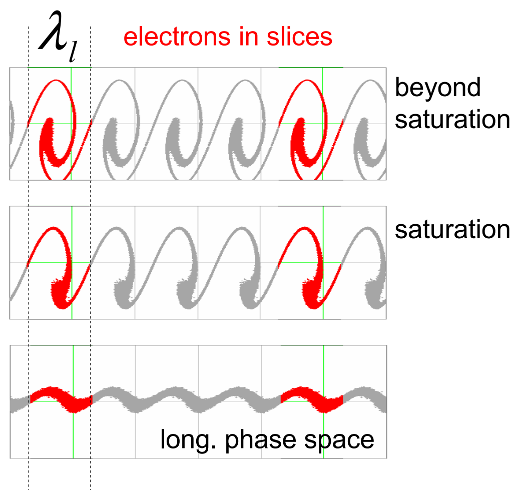
SASE: macro particles with controlled shot noise

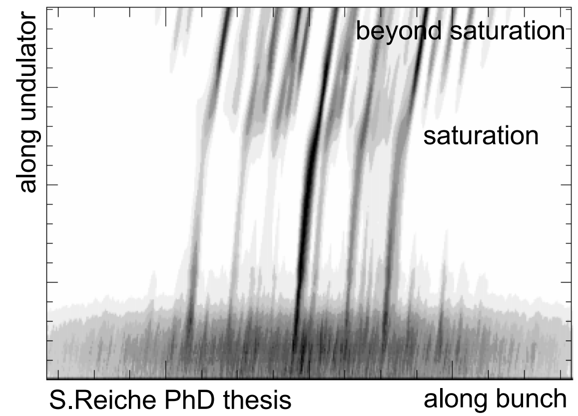
SASE simulation











example: European XFEL, 1nC, 0.1nm

length along undulator = 135 m

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

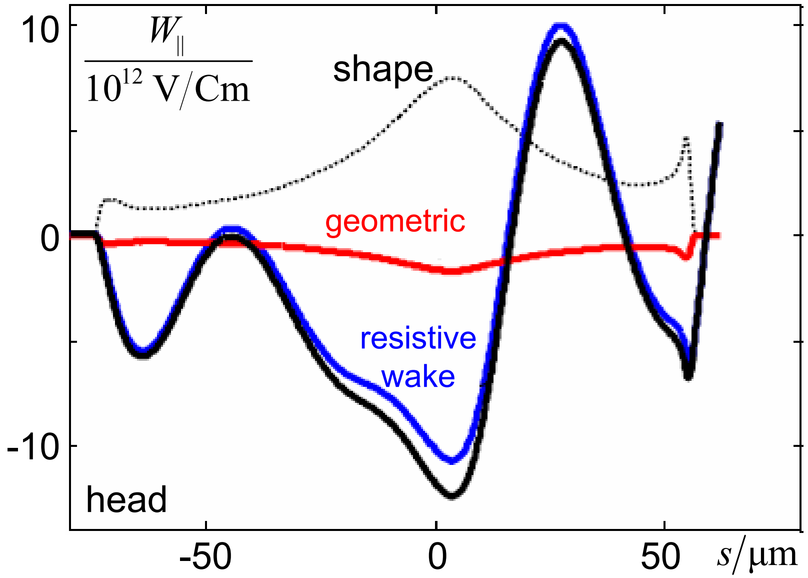
step along bunch: $64\lambda_l$ number of slices ~ 10000

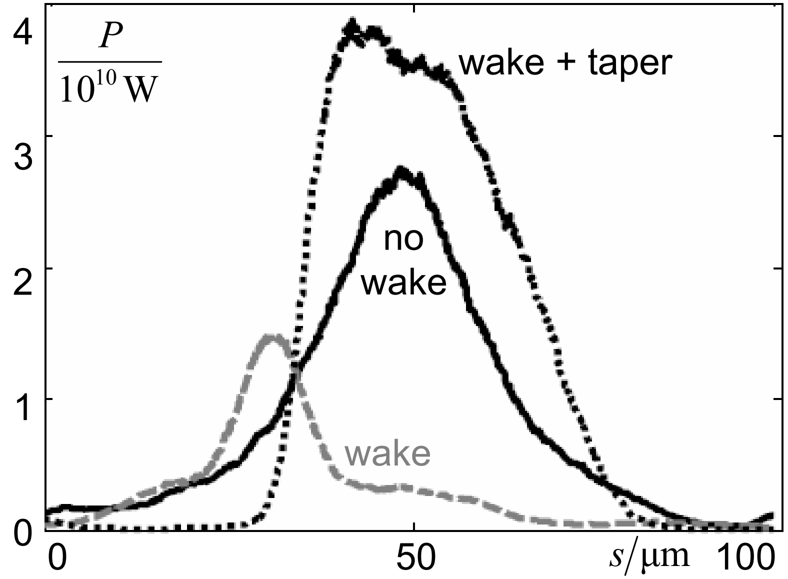
90 min / seed 150 seeds $\rightarrow$ ~ 10 days

LINUX cluster with 20 cpus (64 bit)

Igor Zagorodnov

bunch shape and
different contributions
to long. wake in undulator



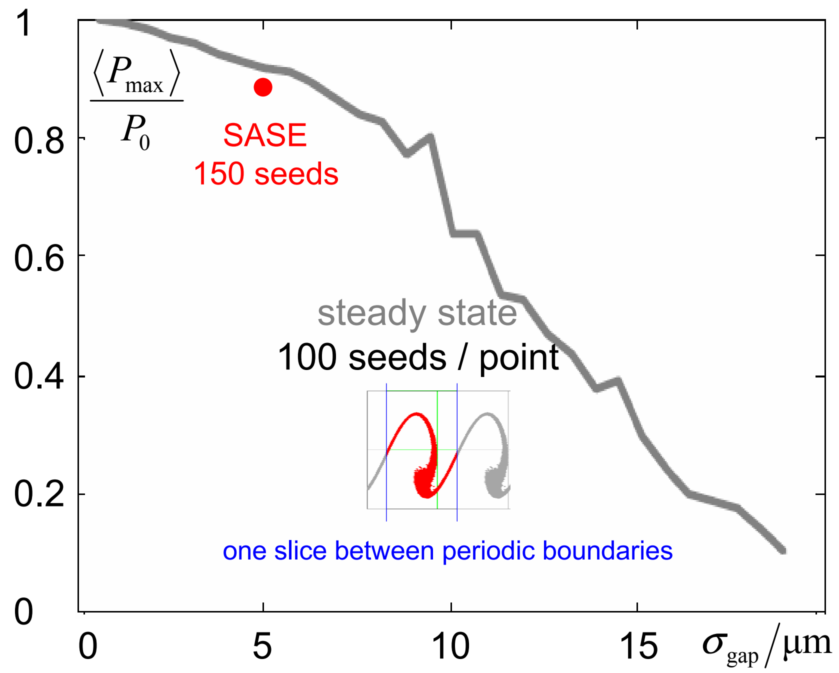


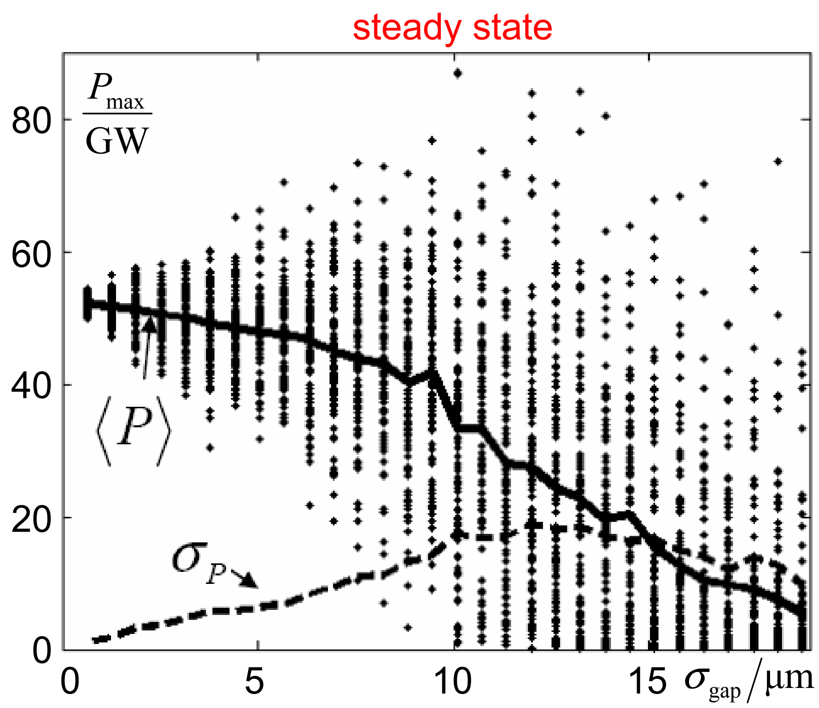
$$\lambda_l = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2}\right)$$

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 / → ~ 1 h all points → ~ 1 day

SASE 90 min / seed 150 seeds → ~ 10 days

PC (32 bit), 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
- change of phase space description
- use of different methods and codes (SC, CSR)
- careful control of computational parameters
- “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)