Parallel Computing in Beam Dynamics Studies for XFEL/FLASH

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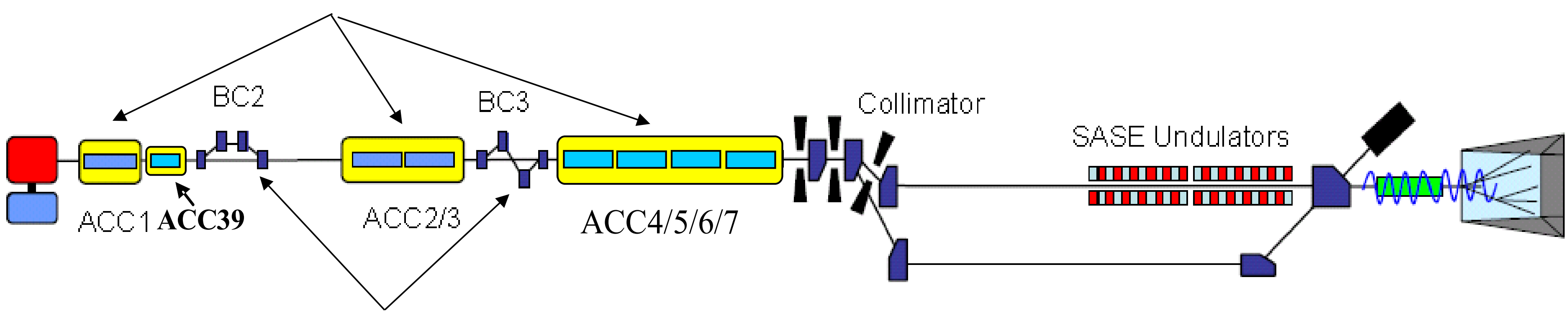
FLASH layout and desired beam parameters

short radiation wavelength $\lambda \sim \frac{1}{\gamma^2}$ ← high electron energy

In accelerator modules ACC1, ACC2,..., ACC7 the **energy** of the electrons is increased from 5 MeV (gun) upto **1200 MeV** (undulator).



In compressors **the peak current *I*** is increased from 1.5-50 A (gun) to **2500 A** (undulator).

short gain length $L_g \sim \frac{\varepsilon^{5/6}}{\sqrt{I}}\left(1 + O(\sigma_E^2)\right)$ (for the optimal beta function)

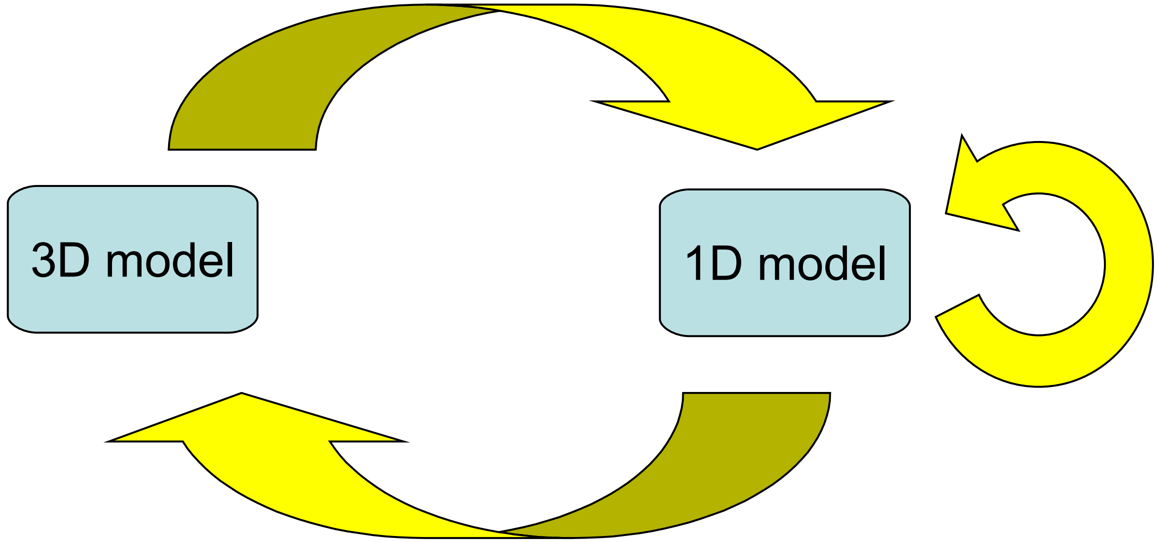
high peak current

3D and 1D simulations with self fields

space charge +cavity wakes + self fields in BCs

1D model was checked through 3D.
Working points are found by optimization in 1D and then checked by 3D.
Finally, 1D model is used to estimate the RF tolerances.

3D results to fit the 1D model

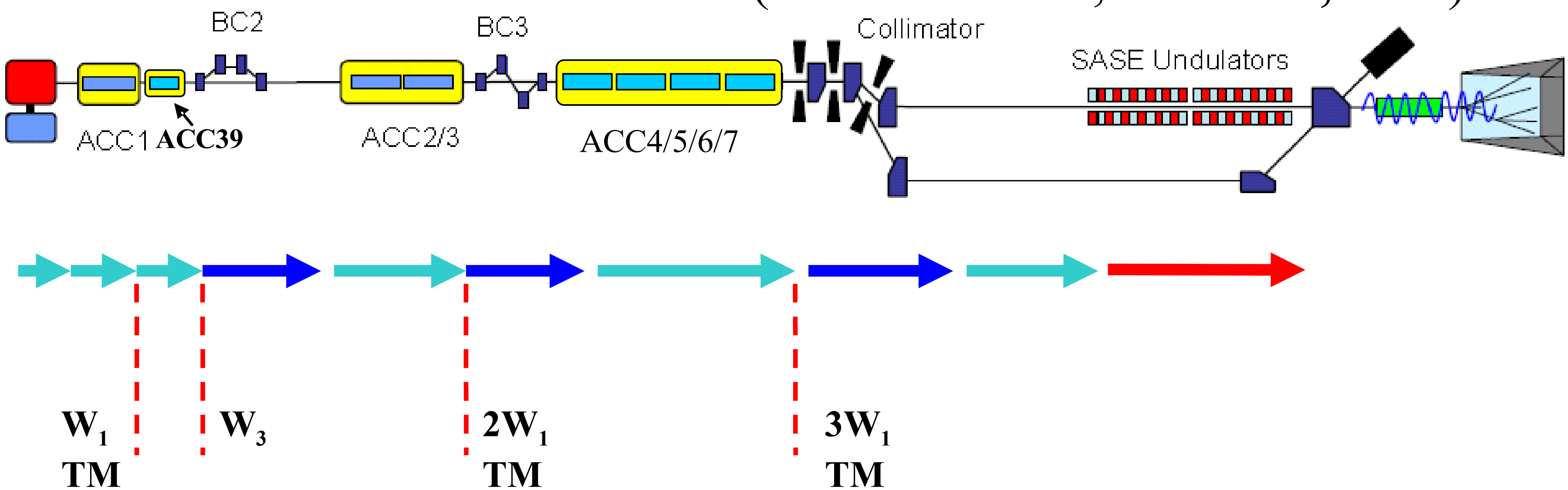


1D scan to find the working point

1D results to use in the 3D model

FLASH beam dynamic simulations for different charges

3d simulation method (self-consistent, **46 CPU ,~10h**)



ASTRA (tracking with space charge, DESY, K. Flötmann)

CSRtrack (tracking through dipoles, DESY, M. Dohlus, T. Limberg)

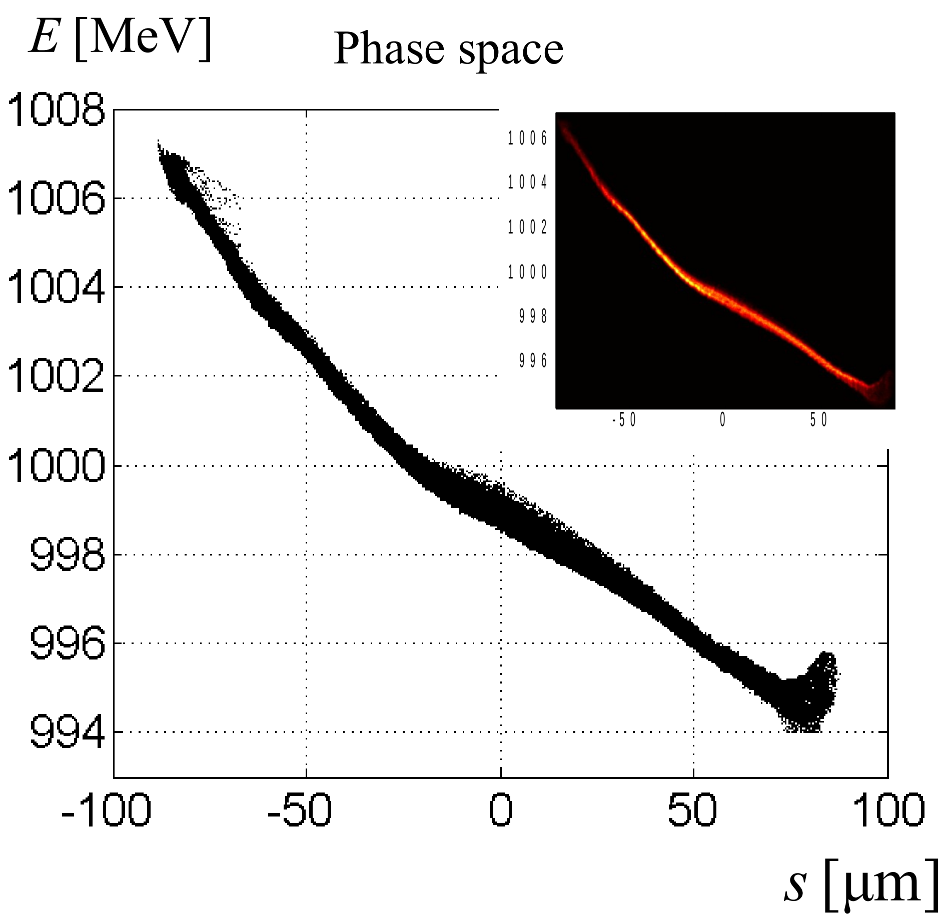
ALICE (3D FEL code, DESY, I. Zagorodnov, M. Dohlus)

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

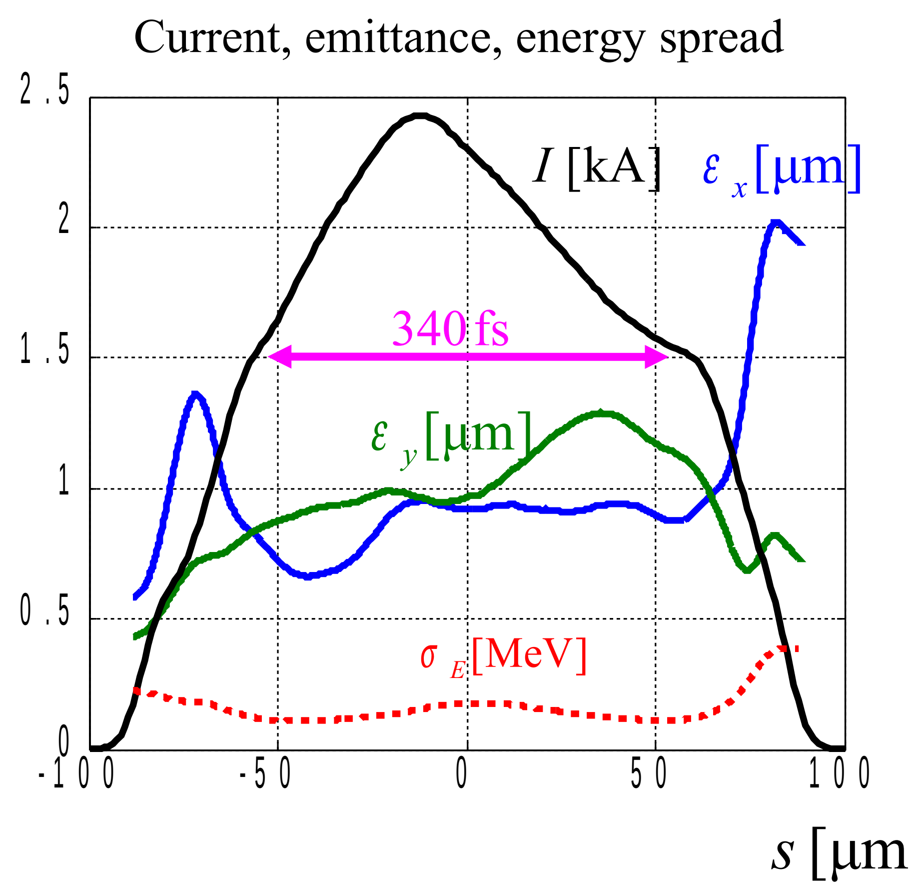
W3 - ACC39 wake (TESLA Report 2004-01, DESY, 2004)

TM - transverse matching to the design optics

FLASH beam dynamic simulations for different charges (Q=1 nC)



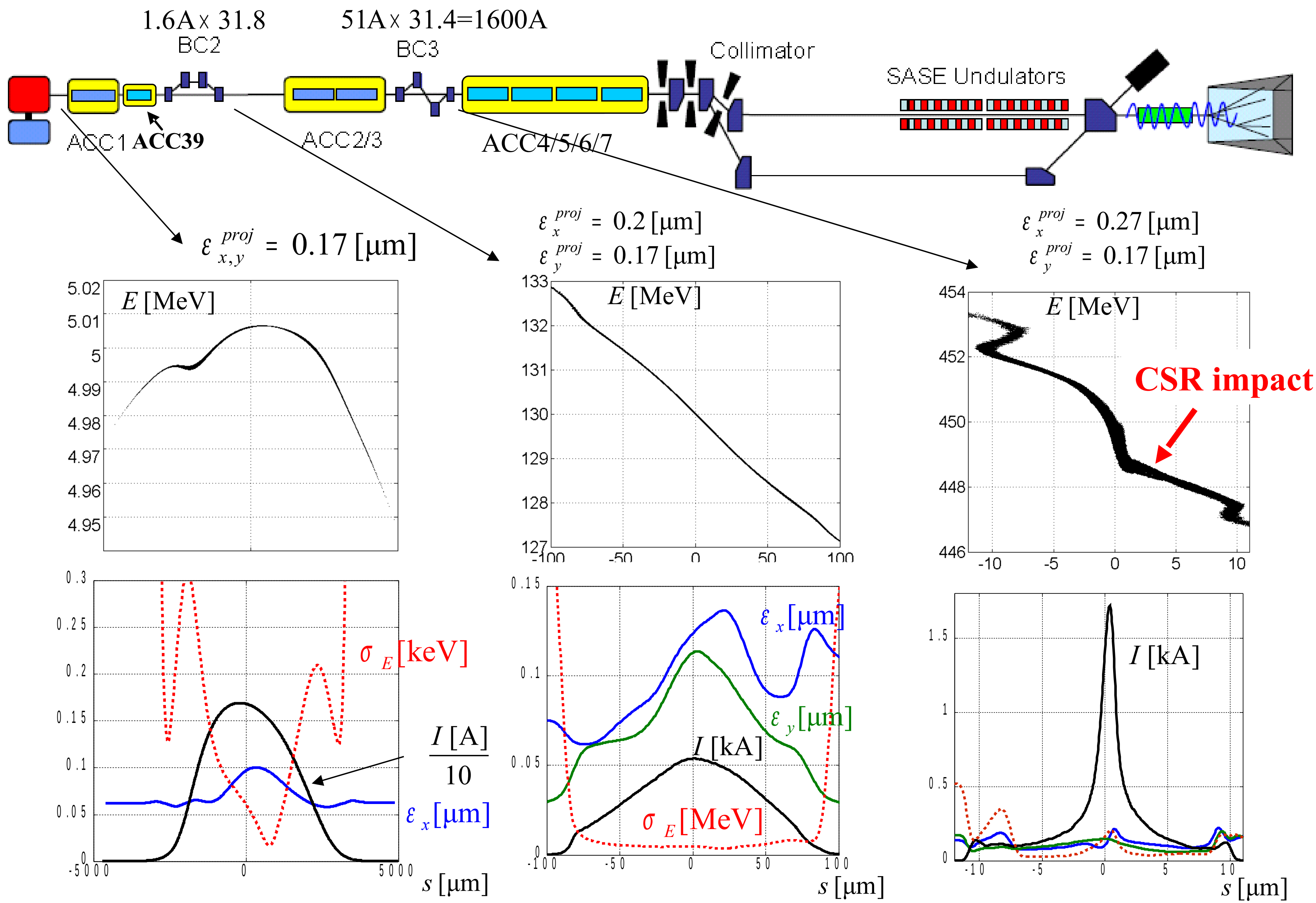
bunch head



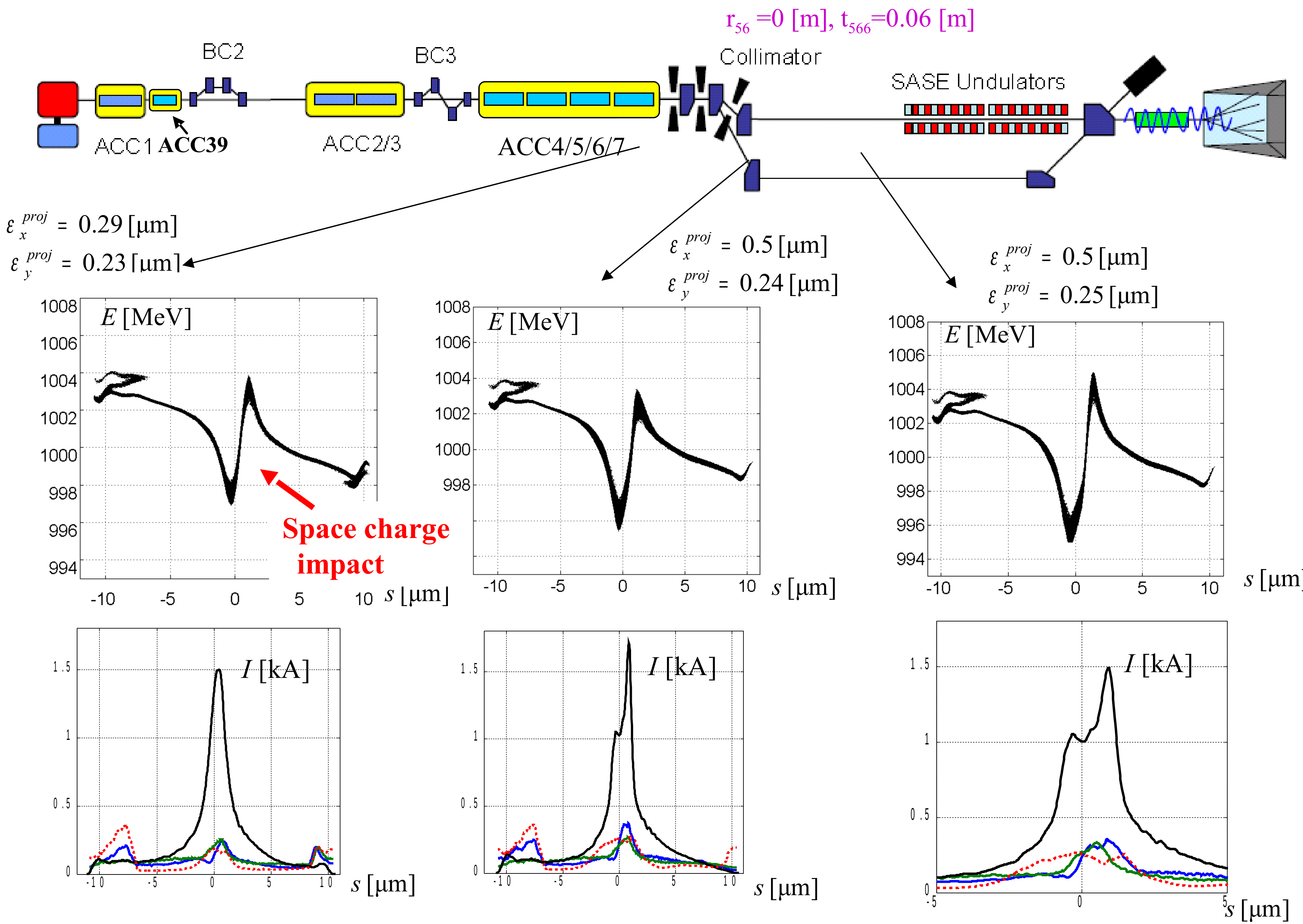
$\varepsilon_x^{proj} = 3\ [\mu m]$

$\varepsilon_y^{proj} = 1.4\ [\mu m]$

FLASH beam dynamic simulations for different charges (Q=0.02 nC)

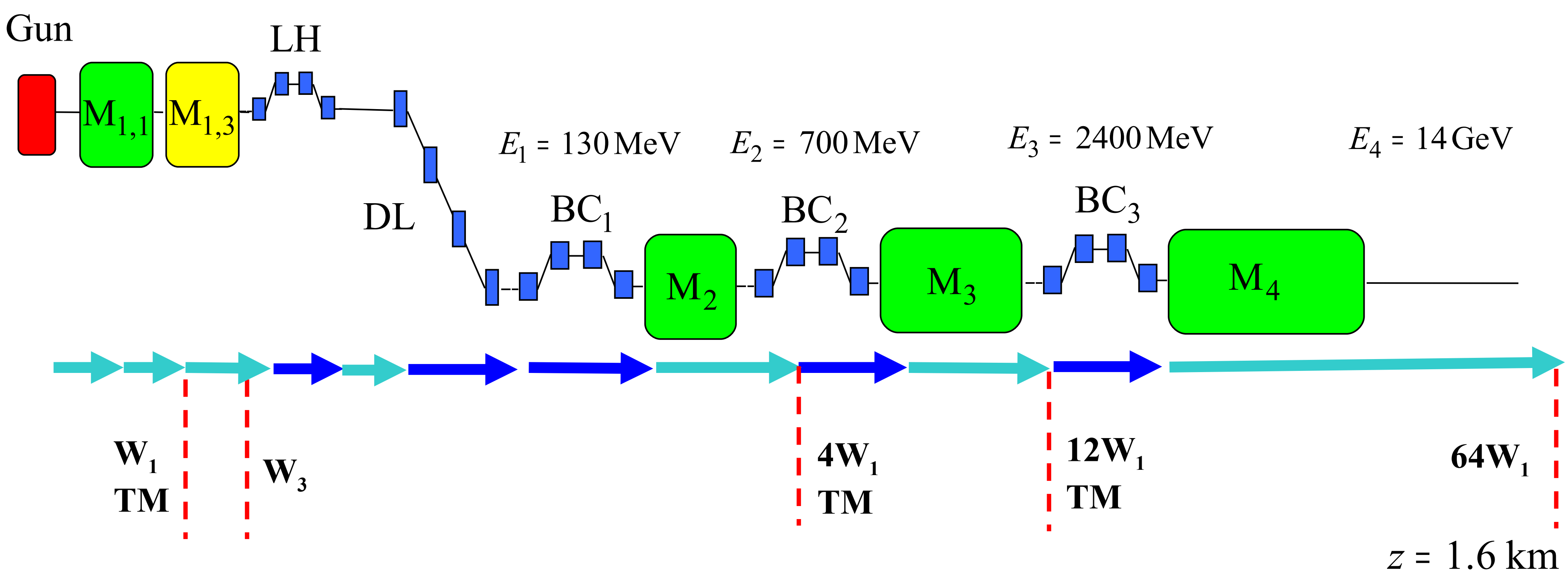


FLASH beam dynamic simulations for different charges (Q=0.02 nC)



Beam dynamics simulations for the European XFEL

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



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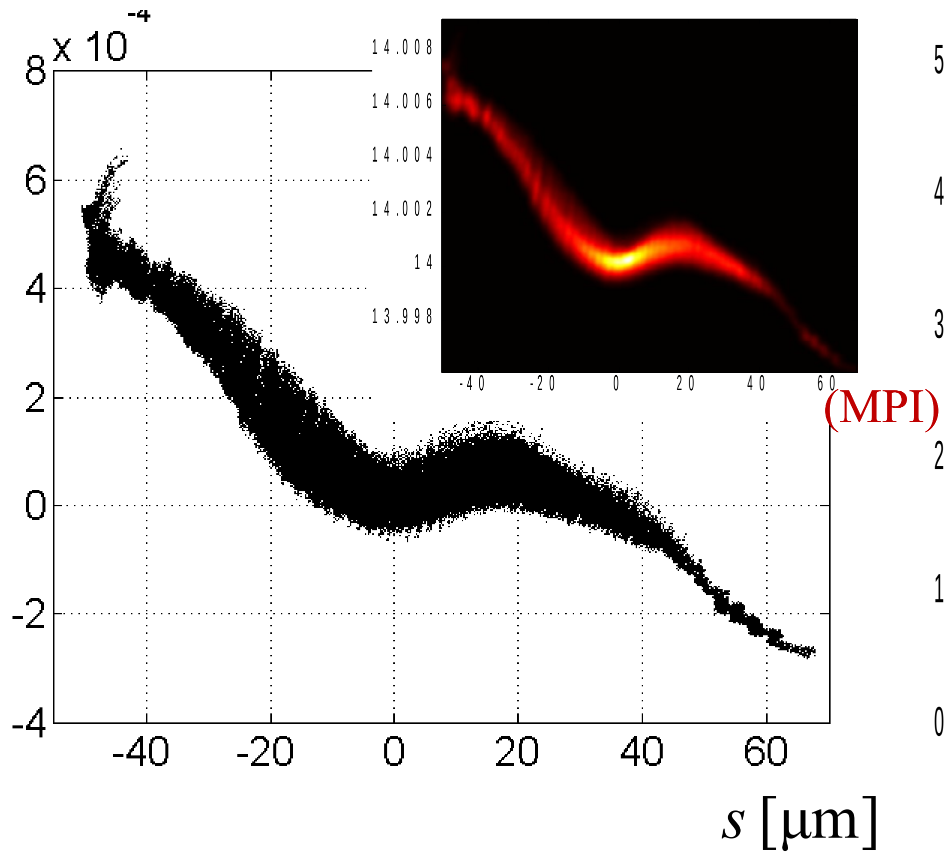
TM - transverse matching to the design optics

XFEL beam dynamic simulations for different charges (full)

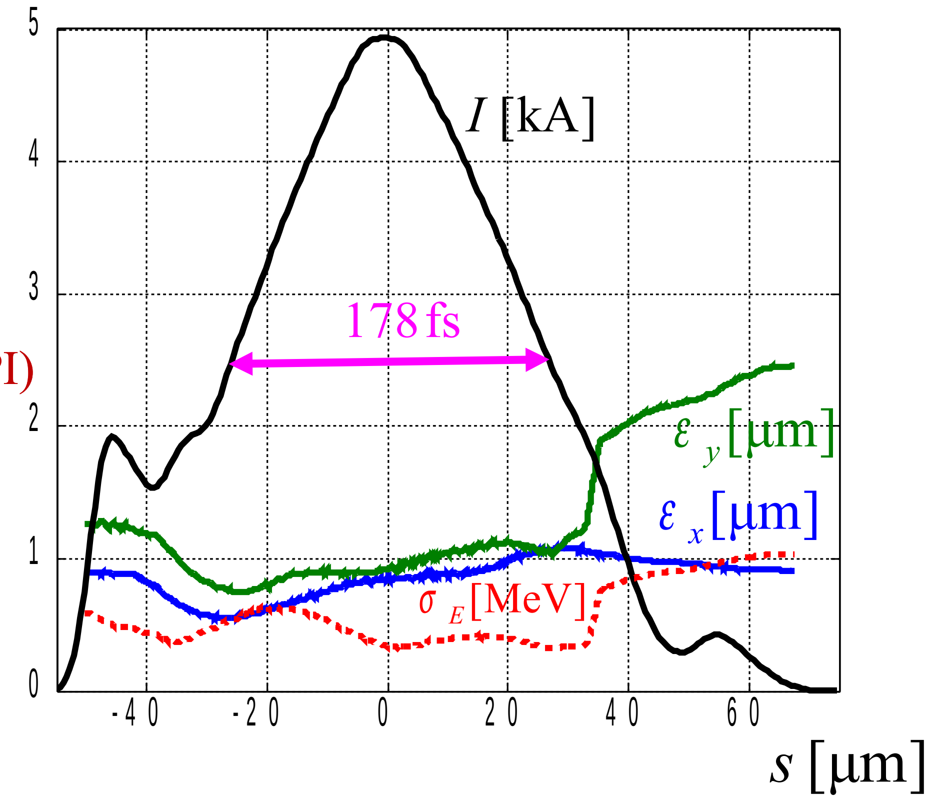
Q=1 nC

δ_E Phase space



bunch head

Current, emittance, energy spread



$\varepsilon_x^{proj} = 0.9$ [µm]

$\varepsilon_y^{proj} = 3.5$ [µm]

We have removed 6% of bad particles in the analysis

Radiation properties for different charges

How to provide (1) a well conditioned electron beam and (2) what are the properties of the radiation?

(1) Self consistent beam dynamics simulations.

We are able to provide the well conditioned electron beam for different charges.

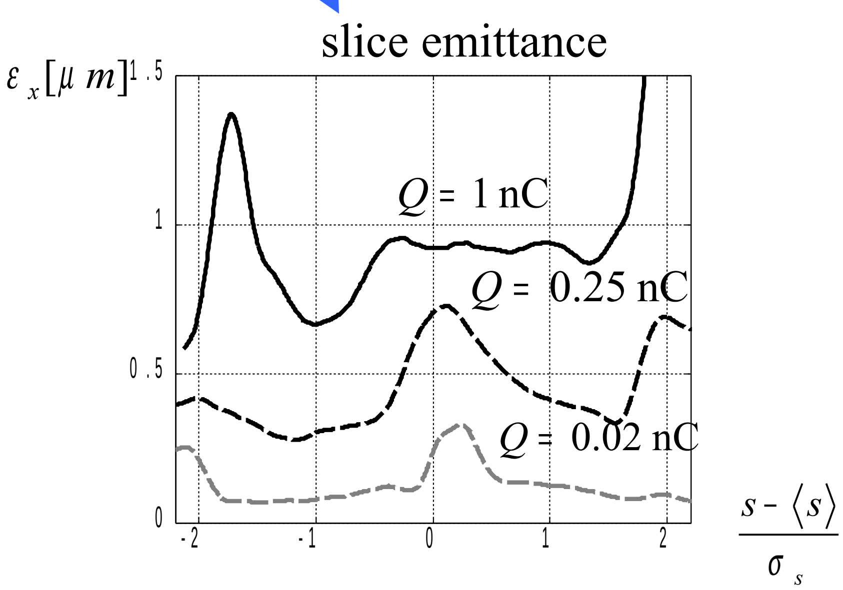
But RF tolerances for low charges are tough.

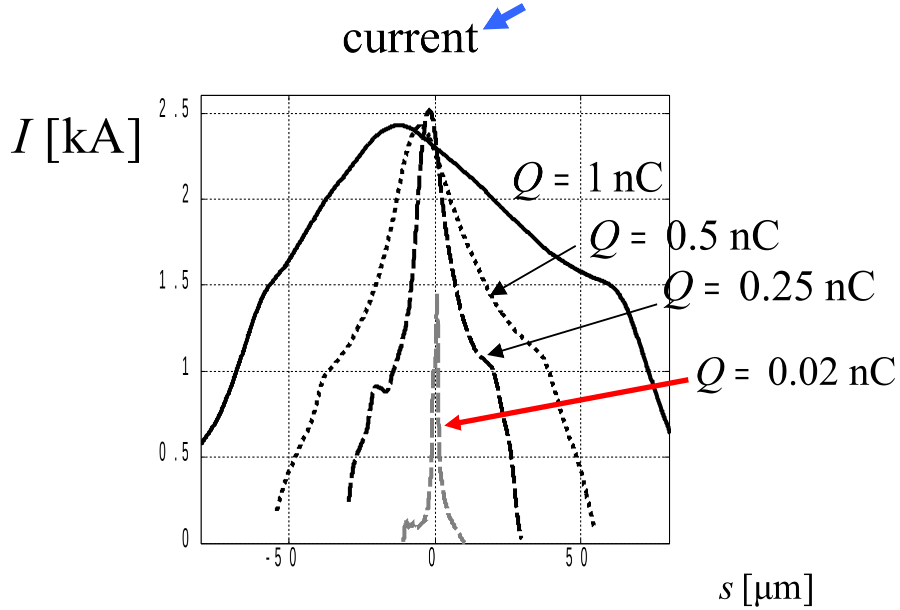
(2) FEL simulations (next slides).

Radiation properties for different charges

Slice parameters are extracted from S2E simulations for SASE simulations

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



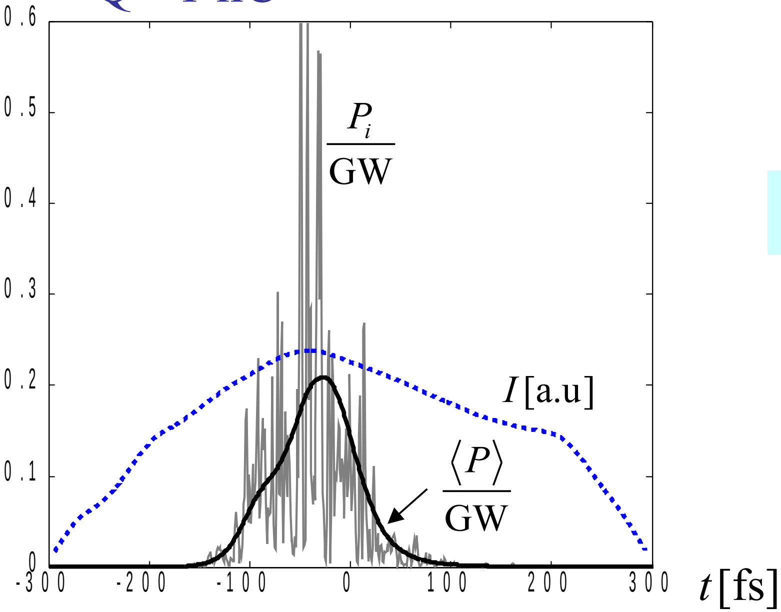


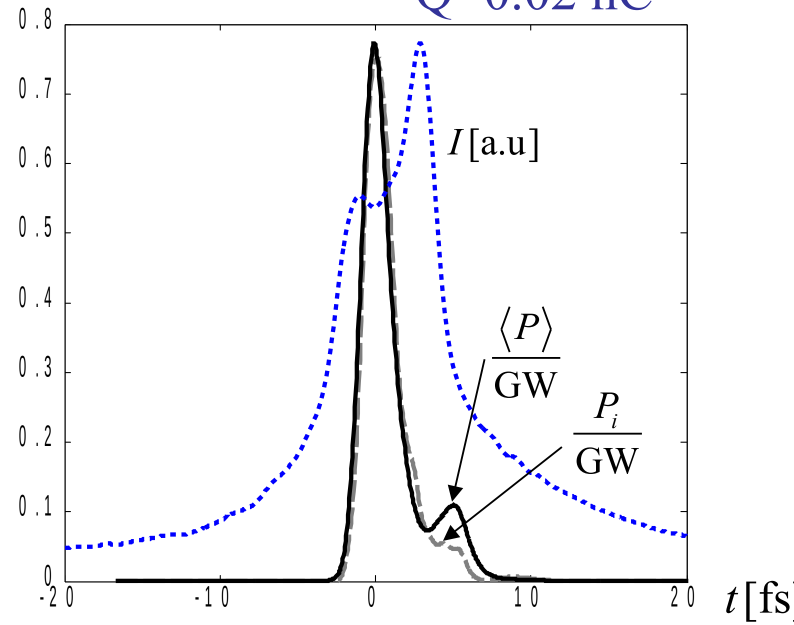
Charge Q, nC	1	0.25	0.02
Longitudinal electron beam size σ_s, μm	42	13	3.6
Transverse electron beam size σ_r, μm	80	68	36

Radiation properties for different charges (46 CPU, ~15 min)

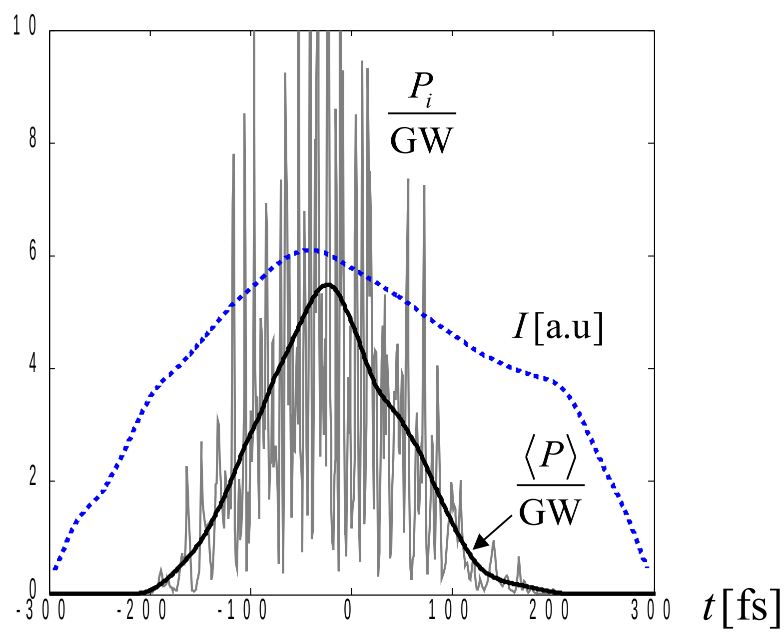
Q= 1 nC

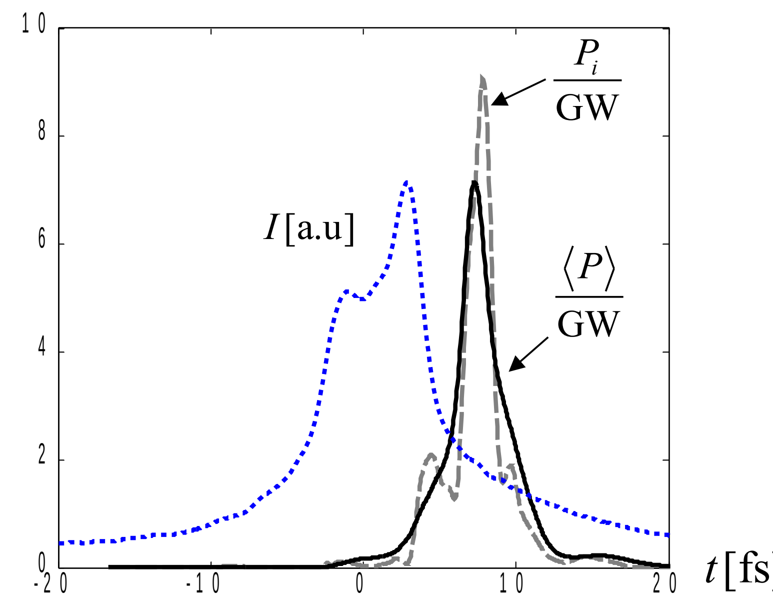
Q=0.02 nC





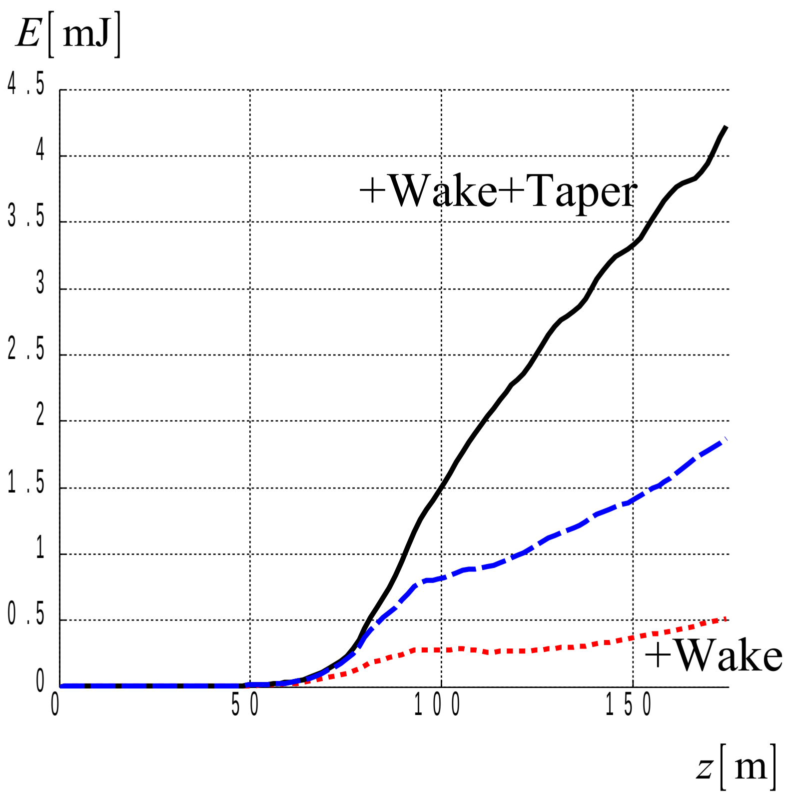
z=10m

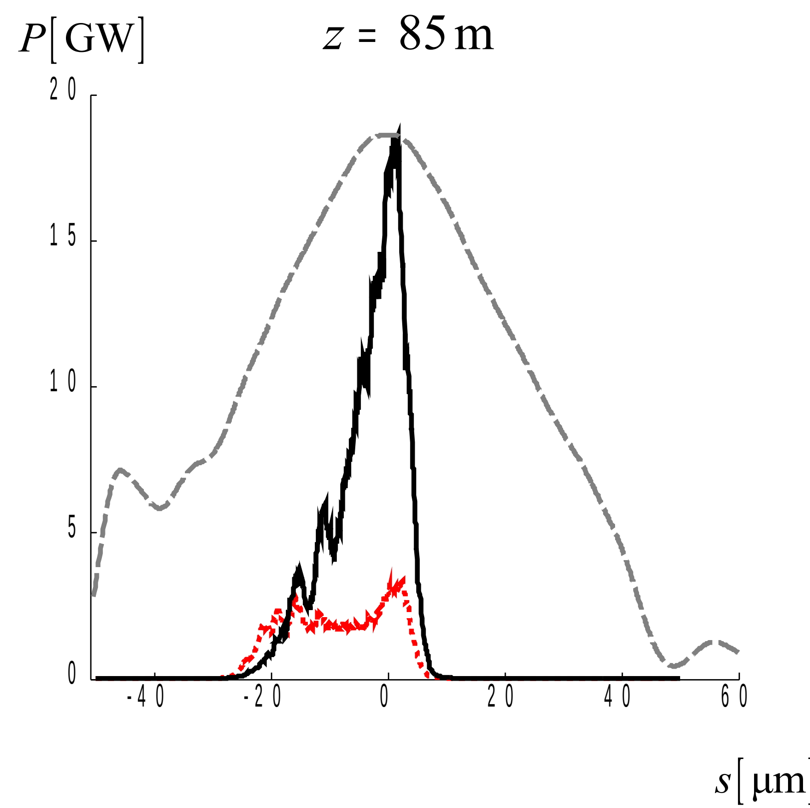




z=20m

SASE radiation Q=1 nC (ALICE, 360 CPU, ~30 min)





Averaged through 8000 slices

FAST: Simulations of FEL physics in the framework of WP21 of the European XFEL

- The FEL operation is well described in the framework of classical mechanics and electrodynamics:

$$d\vec{p}/dt = \vec{F} = -e\vec{E} - e\frac{\vec{v}}{c} \times \vec{H}$$

$$\vec{p} = m_{\mathrm{e}}\gamma\vec{v}, \qquad \vec{H} = \vec{\nabla} \times \vec{A}, \qquad \vec{E} = -\vec{\nabla}\phi - \frac{1}{c}\frac{\partial\vec{A}}{\partial t}$$

$$\triangle\vec{A} - \frac{1}{c^2}\frac{\partial^2\vec{A}}{\partial t^2} = -\frac{4\pi}{c}\vec{j}$$

$$\triangle\phi - \frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = -4\pi\rho$$

- Maxwell equations and equations of particle motion are solved in a self-consistent way.
- FEL theory reached mature status. A set of analytical methods developed allowing to describe linear mode of the FEL operation, as well as numerical simulation codes allowing to simulate full FEL physics.

E.A. Schneidmiller and M.V. Yurkov

FAST: Simulations of FEL physics in the framework of WP21 of the European XFEL

Tools of FEL physics requiring computers:

-Eigenvalue equation – solution provides description of the properties of the beam radiation modes (eigenvalues, eigenfunctions). Currently there are no specific requirements, and (standard) scalar processor can be used.
-Initial value problem – solution provides description of the linear stage of amplification (evolution of the beam radiation modes under specific initial conditions). – requires construction of simulation codes – multiprocessor environment is highly desirable.
-Nonlinear simulation code – complete description of the FEL process including nonlinear effects – multiprocessor environment is highly desirable.

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FAST: Simulations of FEL physics in the framework of WP21 of the European XFEL

- FAST is generic name for FEL computing tools which covers different methods for FEL description (eigenvalue problem, initial-value problem, nonlinear simulation code) in the framework of different models (1-D, 2-D, and 3-D, steady-state, time-dependent).
- Application of parallel computing allowed us to make significant breakthrough in FEL simulation: critical problems are simulated with actual number of particles in the electron beam.
- Mainstream of the code development is application of Open MP. Codes run on a dedicated multiprocessor cluster fast. Parallelization of the code is rather effective, and scales nearly linear from NCPUS=2 until maximum NCPUS =16 (4 x Quad Core Xeon X7350, 2.93 GHz, 4 x 16 GB).
- Required CPU time strongly correlates with accuracy of the results and spans from a few hours (draft simulations) to a few months (data base for XFEL users).
- Currently computing power is main factor limiting complexity of physical models.
- Progress of our simulation program strongly depends on NCPUS on a single board.

E.A. Schneidmiller and M.V. Yurkov

FEL code ALICE

- 1D/2D/3D
- 3D azimuthal field solver (Neumann)
- Leap-Frog integrator
- **Perfectly Matched Layer**
- **transverse motion**
- simplified model
- **parallel (MPI)**
- tested on examples from the book of E.L. Saldin at al “The Physics …“, and by comparison with code Genesis 2.0 of S. Reiche

Used simulation codes summary

FAST	ALICE	CSRtrack	Parallel Astra
FEL simulation code	FEL simulation code	CSR effects simulation code	Particle in cell simulations
E.L. Saldin, E.A. Schneidmiller, N.V. Yurkov	I. Zagorodnov and M. Dohlus,	M. Dohlus, T. Limberg	K. Flöttmann, S. Meykopff
OpenMP: only runs efficiently in shared-memory multiprocessor platforms; scales linear	MPI; scales perfect; each slice is independent	Single processor version	MPI; scale factor depends on parameters and grid algorithm; heavy interprocess communication