Simulation and experiments on THz FEL at PITZ

- Overview
- Beam dynamics and experimental results
- THz FEL simulations
- Summary & outlook

Xiangkun Li for the THz team at PITZ
Beam Dynamics Seminar, DESY Hamburg, 25.03.2025

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

Motivation

Accelerator based THz source for pump-probe experiments at the European XFEL

European XFEL (~3.4 km)

PITZ-like accelerator based THz source (~30 m) →

X-ray

THz

Pump & Probe

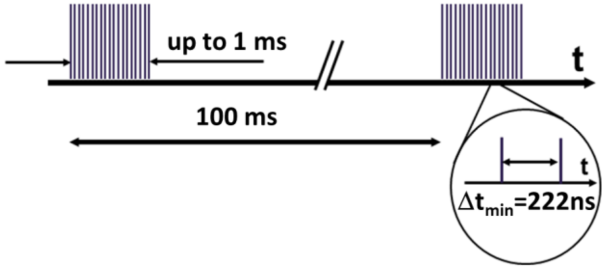
E.A. Schneidmiller, M.V. Yurkov, (DESY, Hamburg), M. Krasilnikov, F. Stephan, (DESY, Zeuthen), "Tunable IR/THz source for pump probe experiments at the European XFEL, Contribution to FEL 2012, Nara, Japan, August 2012

THz source requirements:

- **Tunable** → $f = 0.1 \ldots 20$ THz ($\lambda_{rad} = 3$ mm … 15 μm)
- Various temporal and *spectral* patterns, polarization - ideally **narrow-band** → $\Delta\omega/\omega \sim 0.1 \ldots 0.01$
- **High pulse energy** $W > 10$ μJ (μJ - hundreds of μJ - mJ , depending on f)
- **Time jitter** → from **CEP** (few fs) ***stable*** for field driven to "intensity" driven dynamics (~longest pulse duration) → $\sigma_t \sim 0.1/f$
- **Repetition rate** to follow European XFEL → $(600\ \mu s \ldots 900\ \mu s) \times (0.1 \ldots 4.5\ \text{MHz}) \times 10\text{Hz} = 27000 \ldots 40500$ pulses/s

PITZ Highlights:

- **Identical pulse train** structure as XFEL



- High **charge** feasibility (up to 6 nC)
- Advanced photocathode laser **shaping**
- Initially designed beam for THz FEL
  → **4 nC, 200 A**

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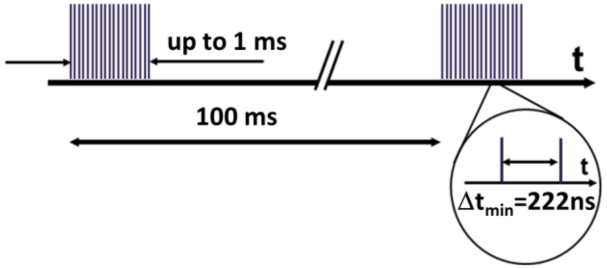
Proposal **"Conceptual design of a THz source for pump-probe experiments at the European XFEL based on a PITZ-like photo injector"** has been supported by the **E-XFEL Management Board** → dedicated R&D activities at PITZ → **Proof-of-principle experiments (2019-2023)**

PITZ Highlights:

- **Identical pulse train** structure as XFEL



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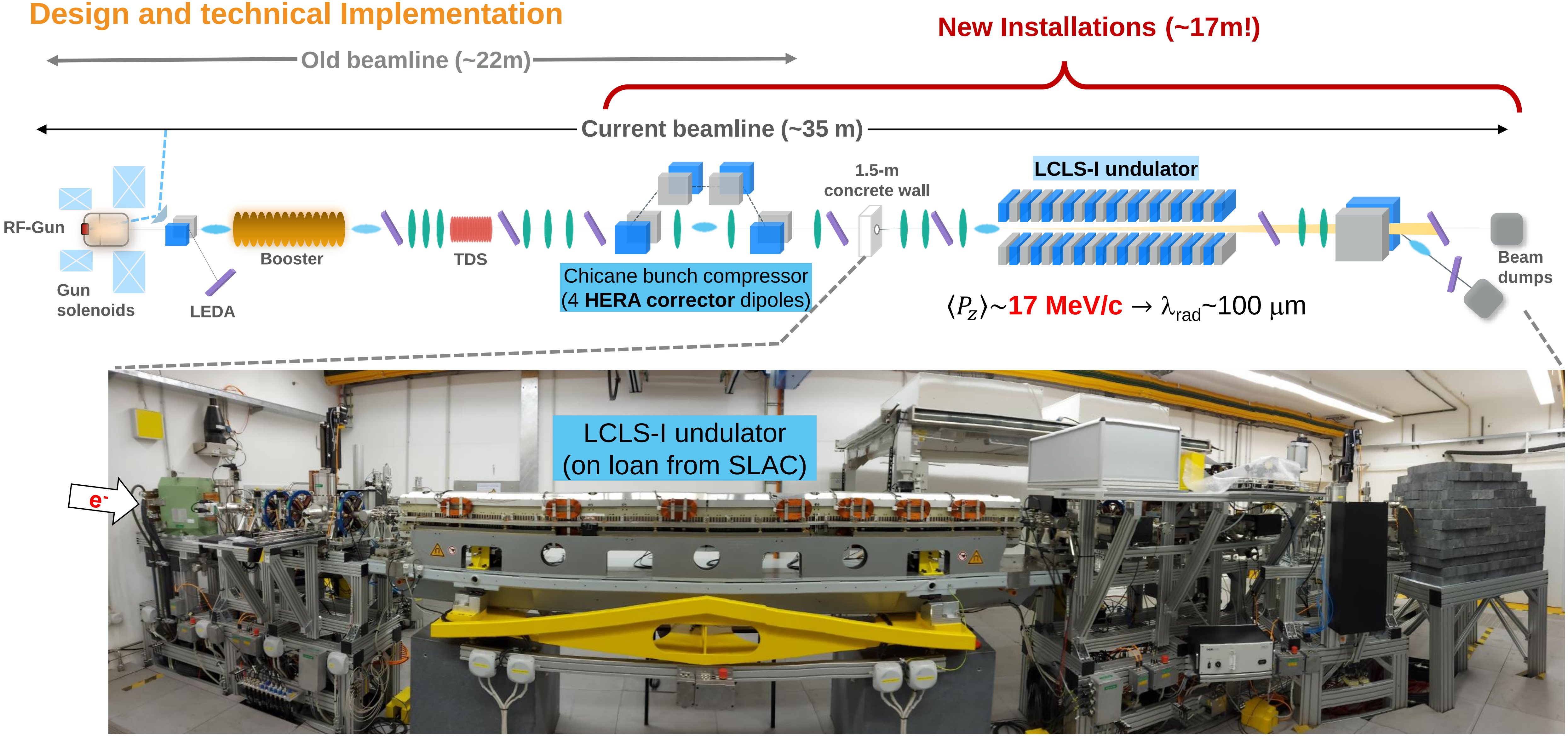
PITZ beamline extension

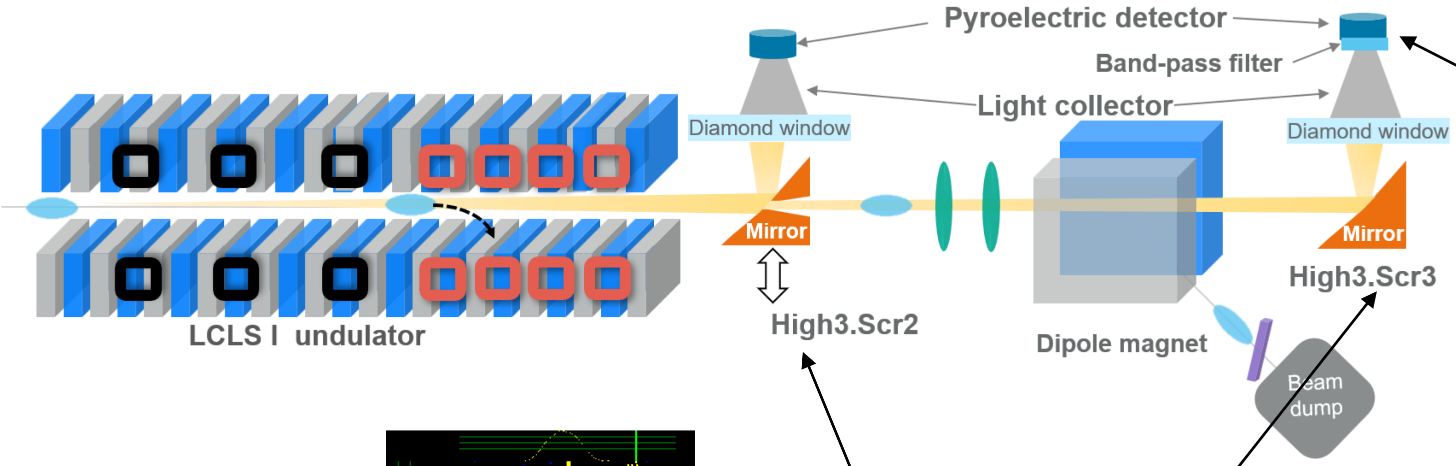
Design and technical Implementation

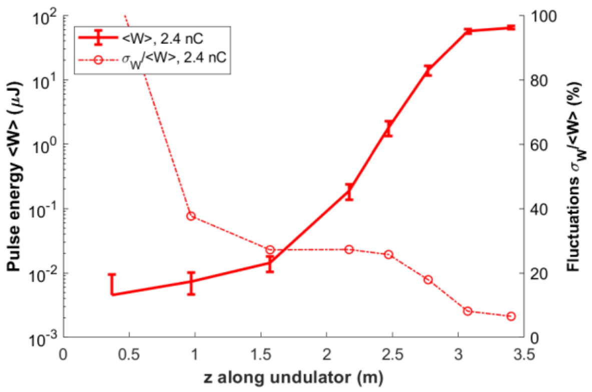


Current status

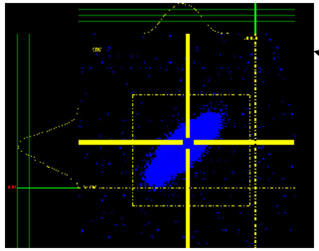
Lasing at ~3THz with ~17MeV/c, ~2nC *Gaussian* beams

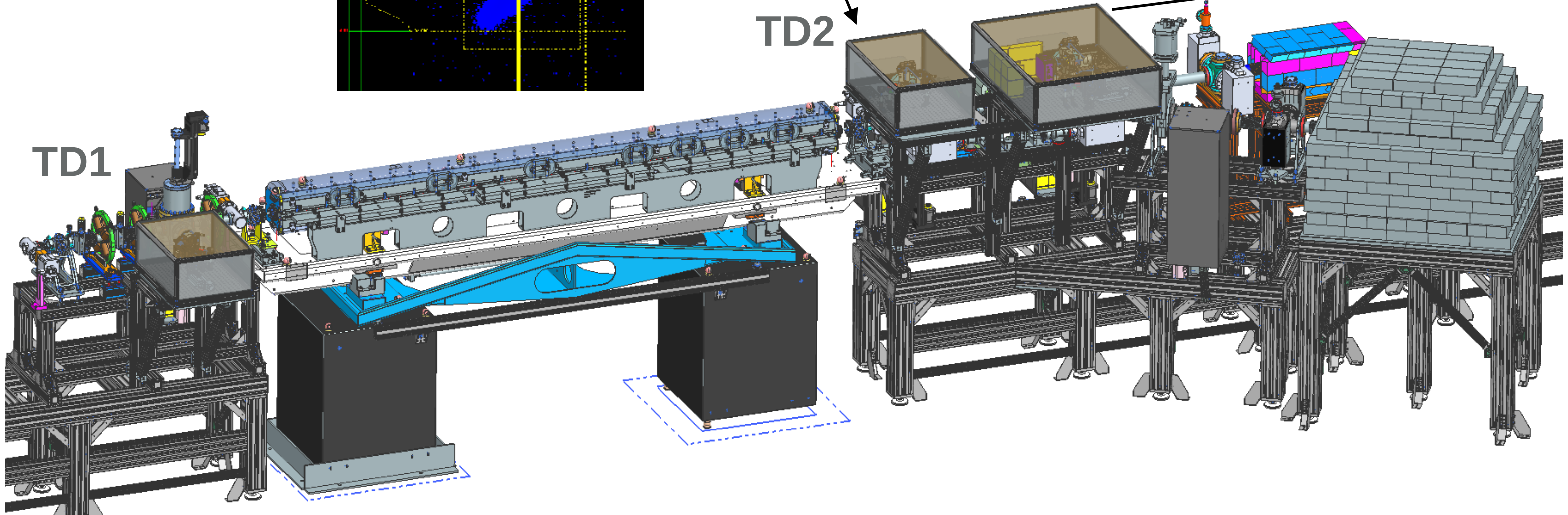
- **Pulse energy:**
  - > 100μJ generated,
  - Energy fluctuations ~6-10%



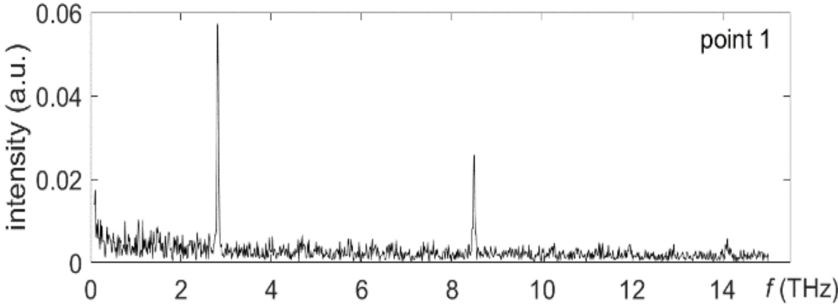


- **THz transverse profile**
  - Focused THz pulse





- **THz spectrum by FTIR (E. Zapolnova)**
  - Narrow (1.7%) bandwidth demonstrated
  - 3rd and 5th harmonics observed
  - $\langle f \rangle = 2.82\,THz$ ($\langle \lambda_{rad} \rangle = 106.5\,\mu m$)



M. Krasilnikov, *et al.*, Phys. Rev. Accel. Beams., 28(3):030701, 2025

Courtesy of N. Aftab

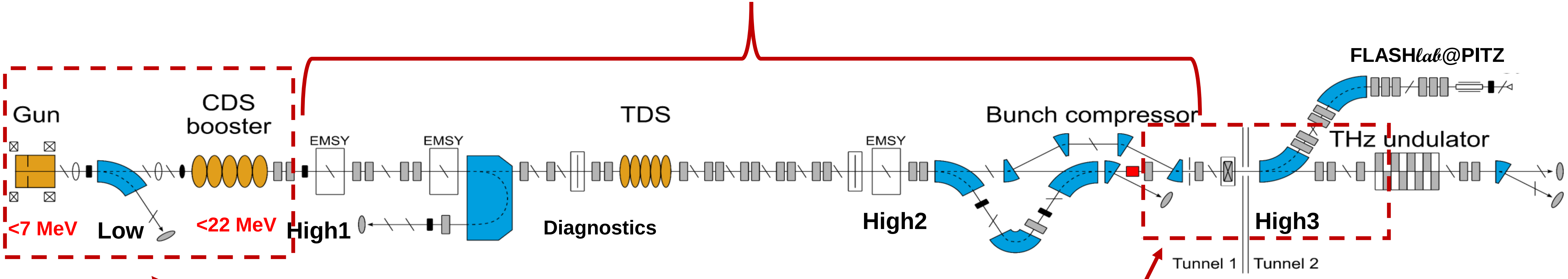
Beam dynamics and experimental results

Beam dynamics overview

Challenge: 2-3 nC 17 MeV/c beam over ~30 m transport and matching into LCLS-I undulator

Transport of electron beam

- Focusing while not spoiling beam quality
- Routine and reproducible procedure



Optimization of photoinjector

- Transverse and longitudinal phase spaces
- Knobs: Laser distributions, Solenoid fields, Booster phase, Steering or beam trajectory

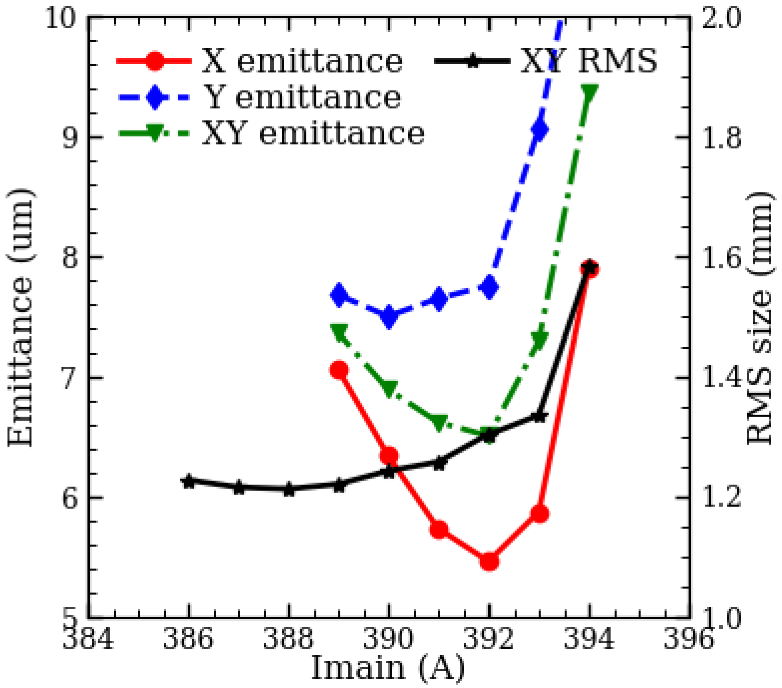
Matching of transverse phase space

- At undulator, Chicane, …
- Limited diagnostics + space charge effects
- Matching procedure

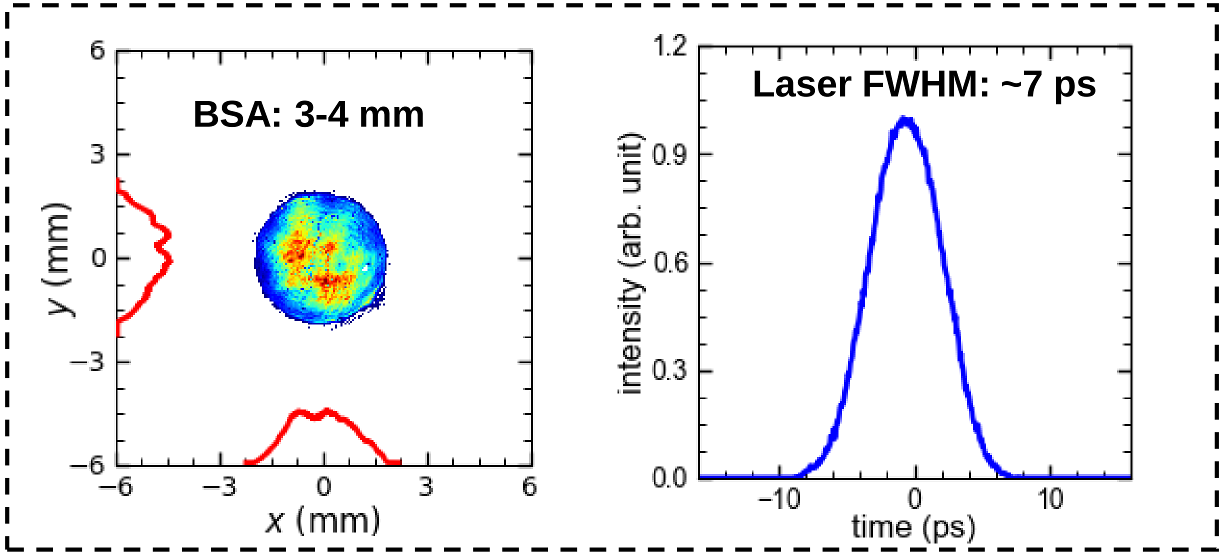
Optimization of photoinjector

Normalized emittance

- Routine emittance optimization
  - Beam shaping aperture (BSA) and solenoid scan



Solenoid scan for emittance optimization (4 nC)
(compared to Astra simulations of ~4 mm mrad)

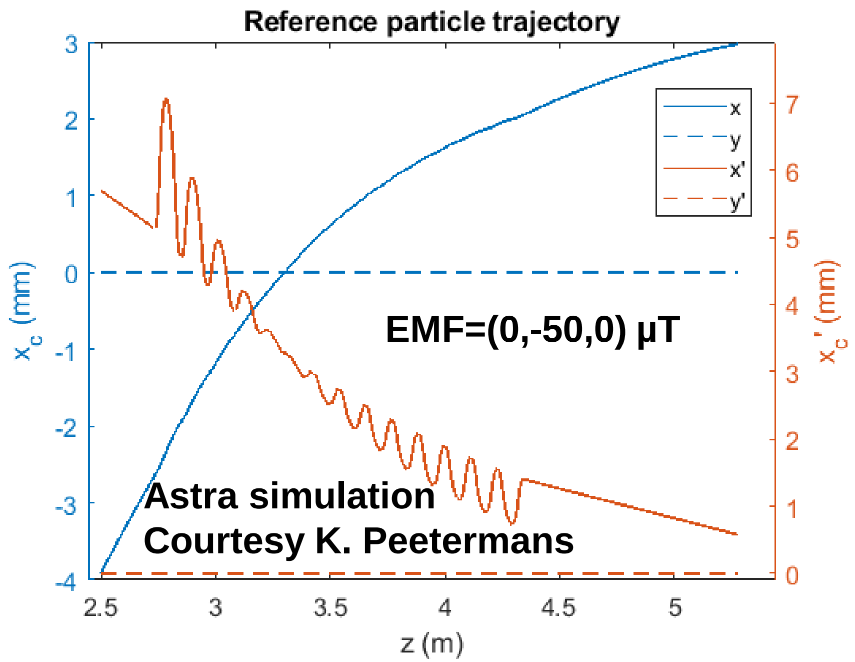


- Up to now, Gaussian photocathode laser was used in experiments
- 20 ps flattop laser is now available from NEPAL laser, hopefully to improve the beam quality and THz output

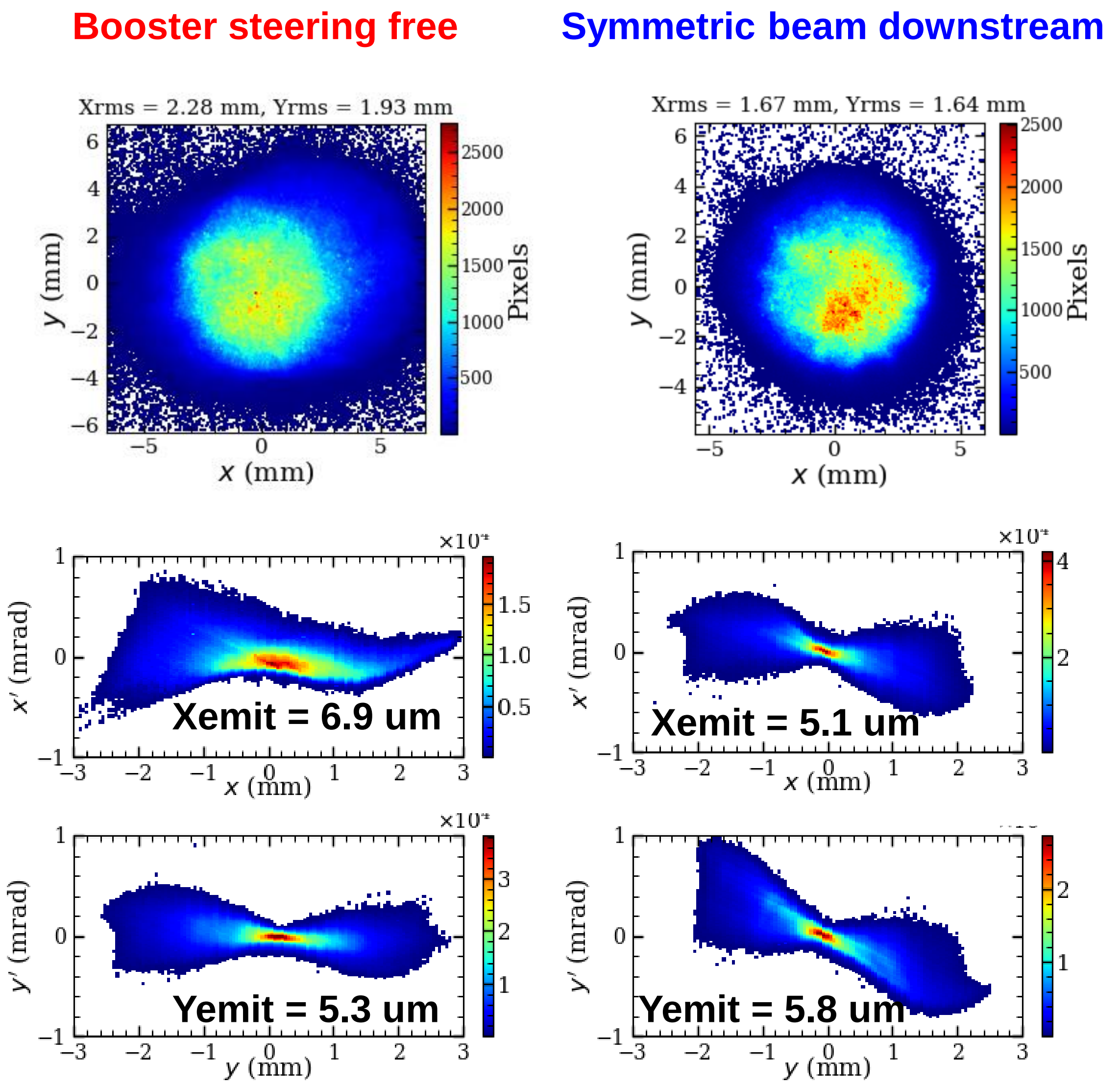
Optimization of photoinjector

Phase space and trajectory

- Measured emittance (phase space) also depends on
  - Laser alignment in the gun (laser BBA)
  - Gun quadrupoles (quadrupole field from solenoid)
  - **Beam trajectory** in the booster (booster BBA)



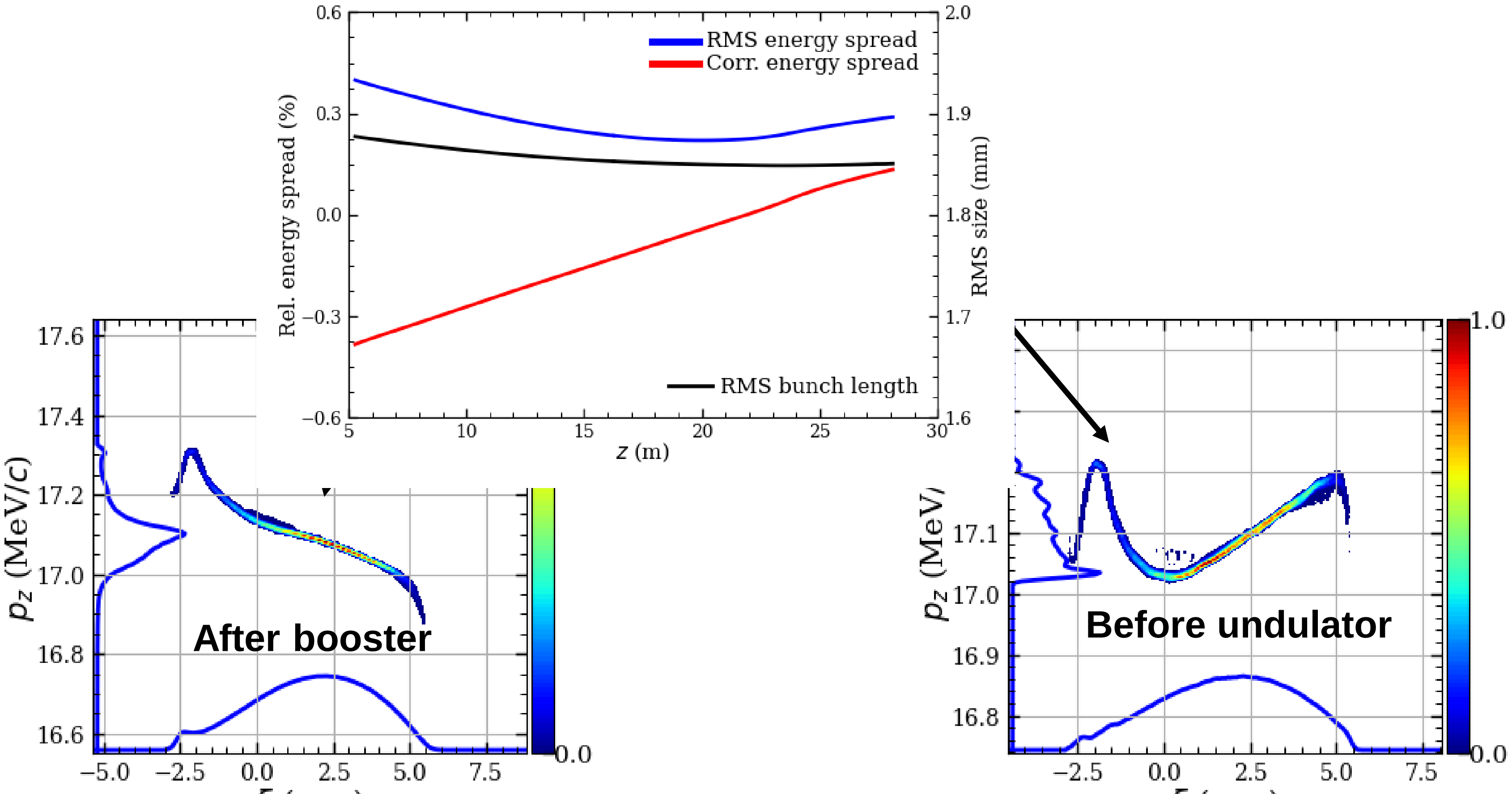
Earth's magnetic fields → off-axis trajectory → wakefields



Optimization of photoinjector

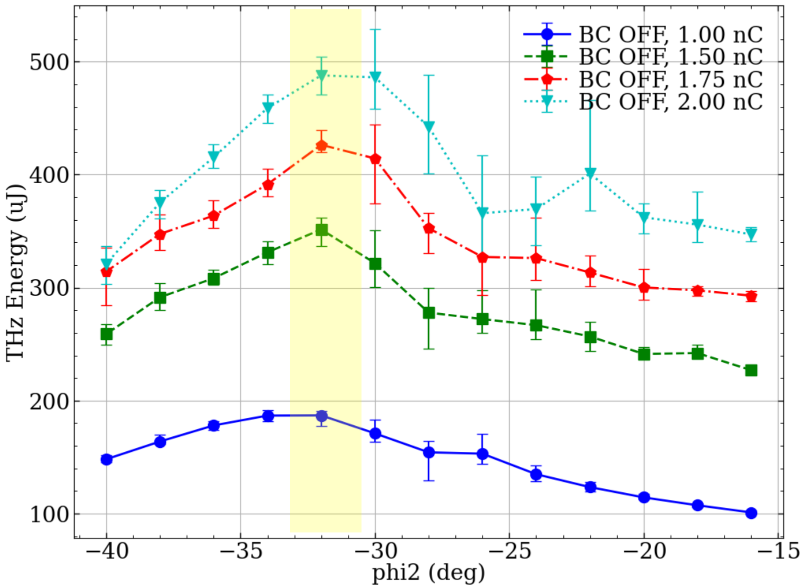
Longitudinal phase space (LPS)

- The RF phases in the gun and the booster can be tuned for optimizing the LPS
- Booster phase → control **LPS** & the **peak current** → maximize THz output



Astra simulation

THz Energy vs booster phase



Impact-T/Z and Genesis1.3
Courtesy B. Li

Transport of electron beam

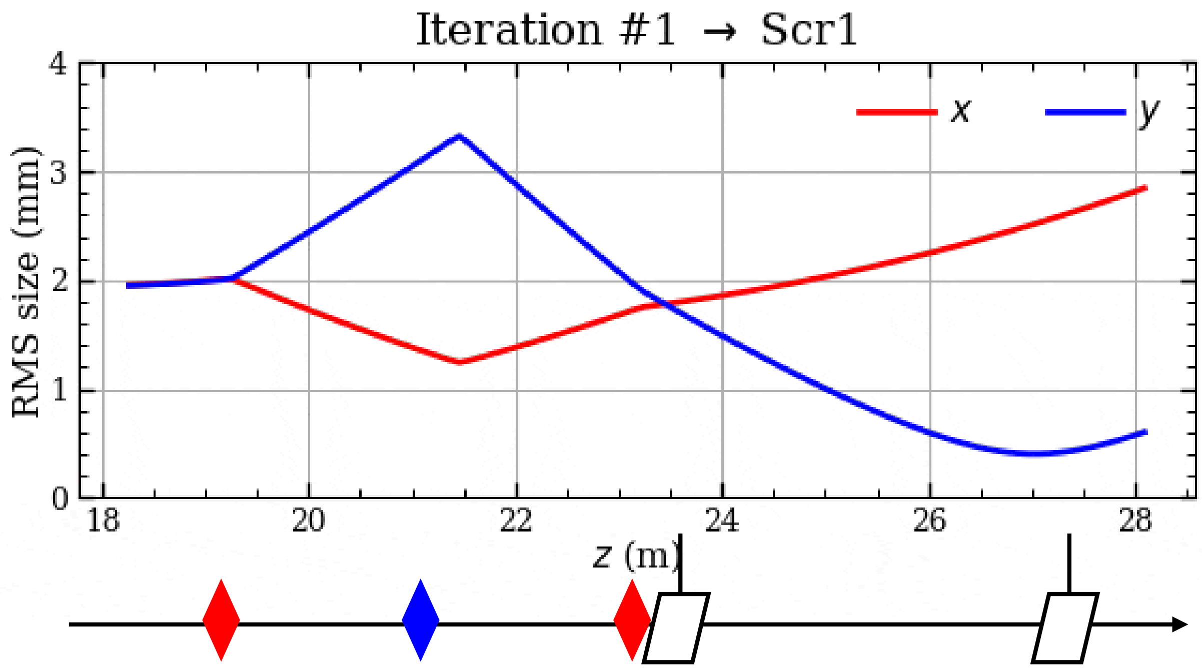
- There is a **long** transport beamline (**~23 m**) from the booster accelerator to the undulator
- The beam size and emittance **grow fast** due to **collective effects** if the beam is not well focused
  - Space charge changes along the bunch slices, causing them to rotate at different rates in the phase space

- A preferred beam transport requires
  - Change of beam size predictable
  - Already found lattice reproducible
  - A well-established and possibly routine procedure
  - If possible, keeping the beam emittance small

Transport of electron beam

Method: symmetric beam transport

- The beam is focused equally in horizontal and vertical plane with quadrupole triplet
- Iteratively increase the amplitude of quad currents **after degaussing → reproducible** magnet setting
  - Beam size at two downstream screens monitored alternatly
- This ensure a **smooth** and **symmetric** beam transport after the triplet, where the beam size cannot be measured everywhere

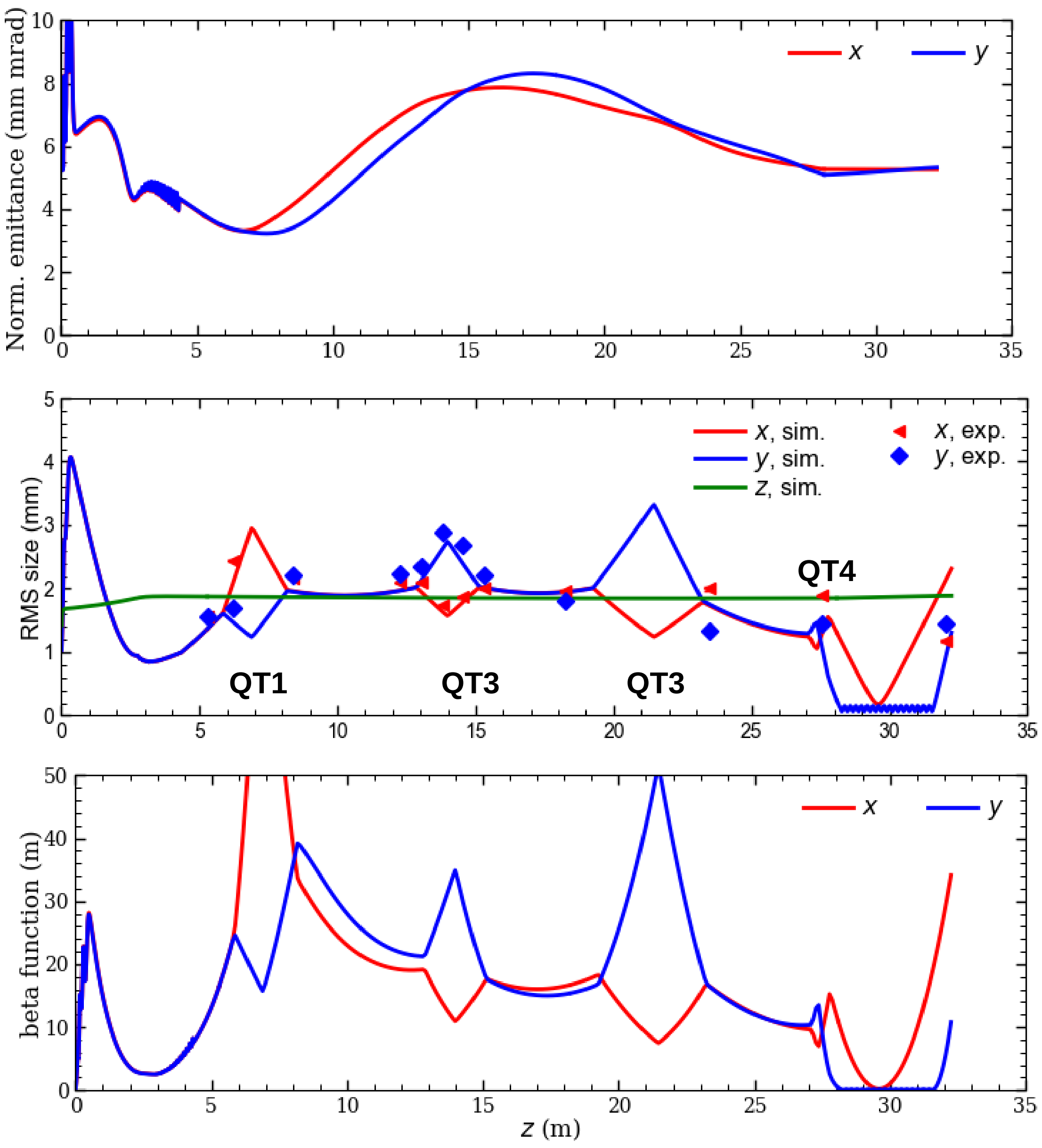


Ocelot simulation

Transport of electron beam

Result

- In total, **four quadrupole triplets (QT)** are used to focus and match the beam from the booster to the undulator
- With the first three triplets, the beam is focused equally in both transverse planes
  - The beam emittance is also controlled by the quadrupoles
- **Note**: no beam optics in the $\phi 36\ \mathrm{mm}$ pipe in the 1.5 m thick concrete **wall ($z \sim 26\ \mathrm{m}$)** between tunnels



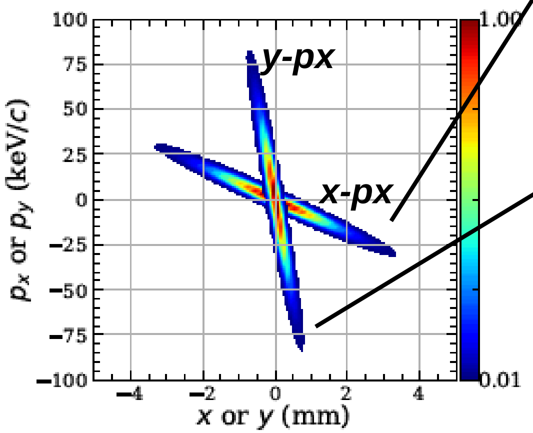
Astra and Ocelot simulation

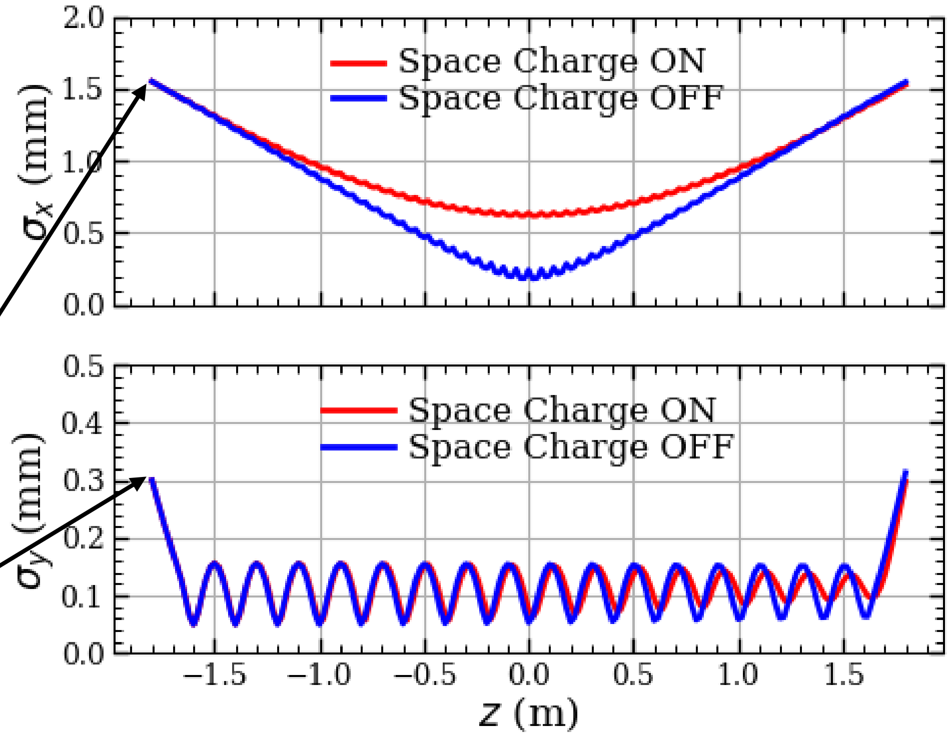
Matching into LCLS-I undulator

- The LCLS-I undulator vacuum chamber (**11 mm x 5 mm, 3.4 m**) is very “small” for **17 MeV/c** electrons
- **Space charge force** and **strong vertical focusing force** (**K~3.5**) from the undulator fields can lead to a rapid growth of the beam size and therefore beam loss, if the transverse phase space is not matched

In the horizontal plane, the motion is dominated by the space charge; in the vertical plane, it is up to the undulator focusing fields

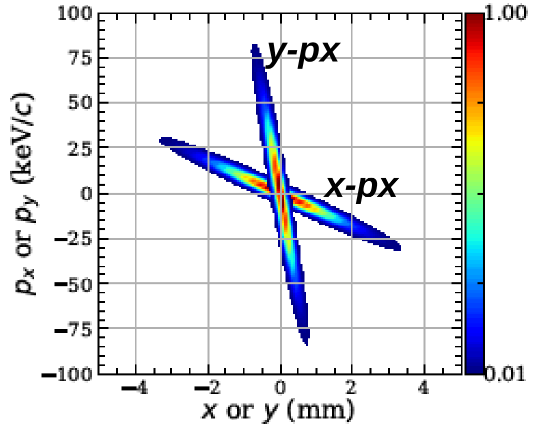
→ **Matched phase space** is defined by independent parameter scan in two planes





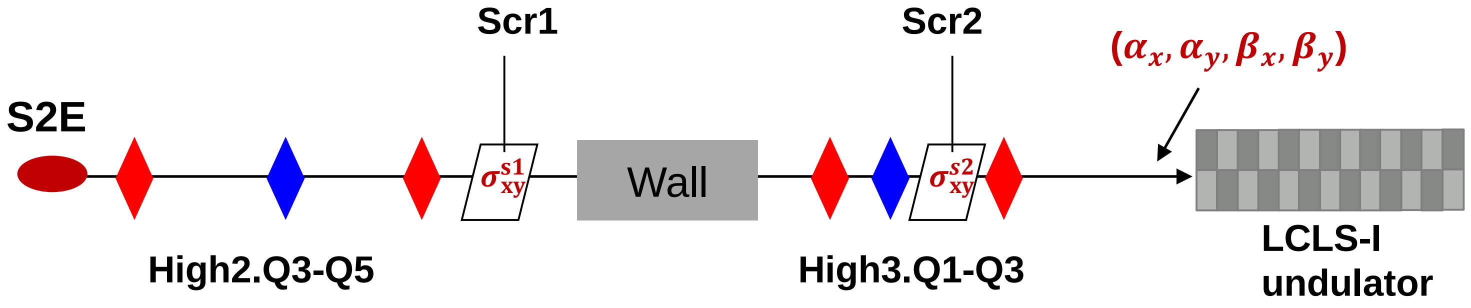
Beam transport in LCLS-I undulator
Astra simulation

Matching into LCLS-I undulator

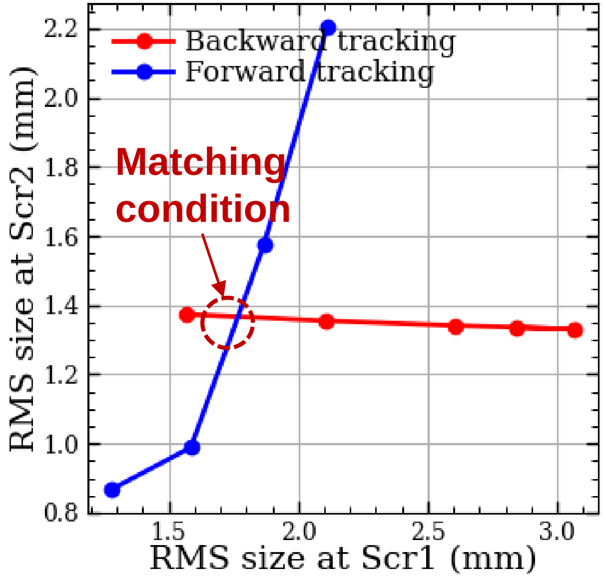


Method

- **Beam envelope** development is determined by matched **Twiss parameters + space charge**
- **Symmetric beam transport:** $\alpha_x, \alpha_y, \beta_x, \beta_y$ **Before undulator** → $\sigma_{xy}^{s1}, \sigma_{xy}^{s2}$ **At two screens**



- Start-to-end simulations define the beam envelope at the two stations
  - **Forward tracking** (scanning of first triplet) → Blue curve
  - **Backward tracking** (scanning of second triplet) → Red curve



Matching simulation (2 nC)

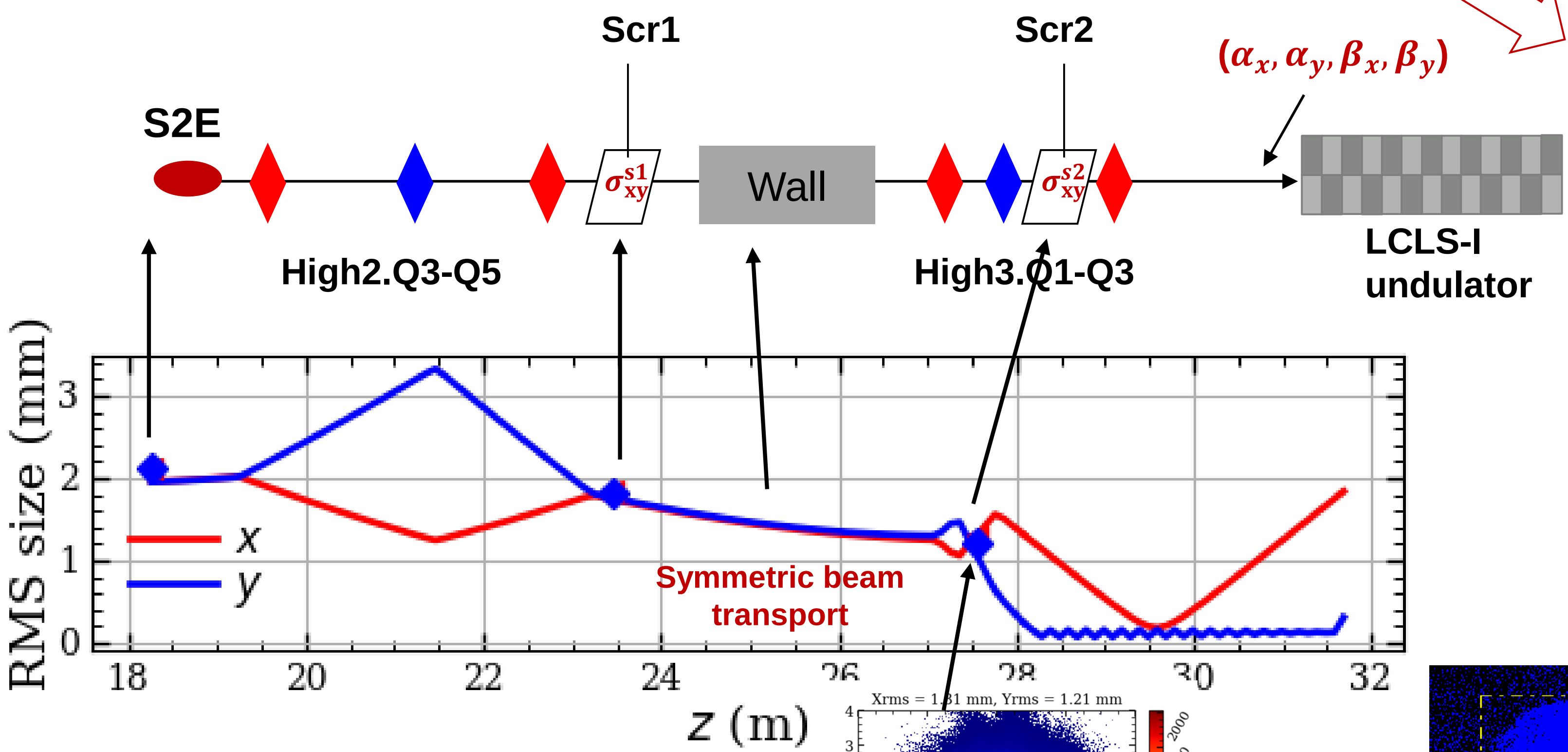
By Ocelot

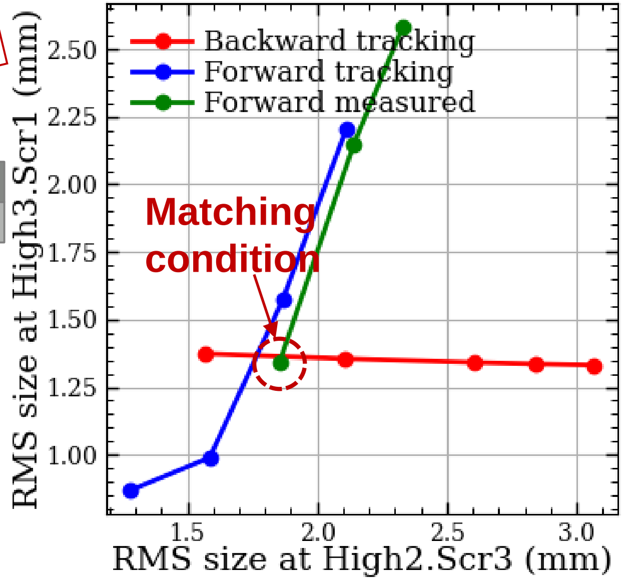
X.-K. Li, *et al.*, *Proc. IPAC'21*, 3244-3247.

Matching into LCLS-I undulator

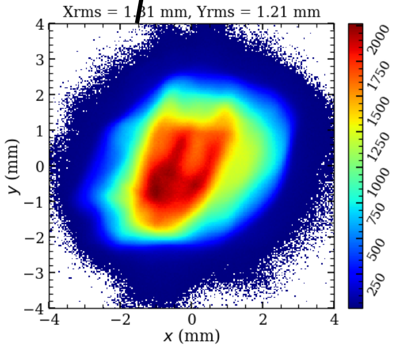
Result

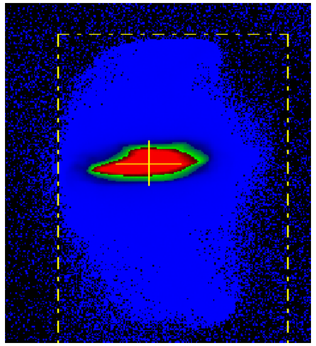
- **Tuning** the first triplet in the **experiments** is like the forward tracking → Green curve





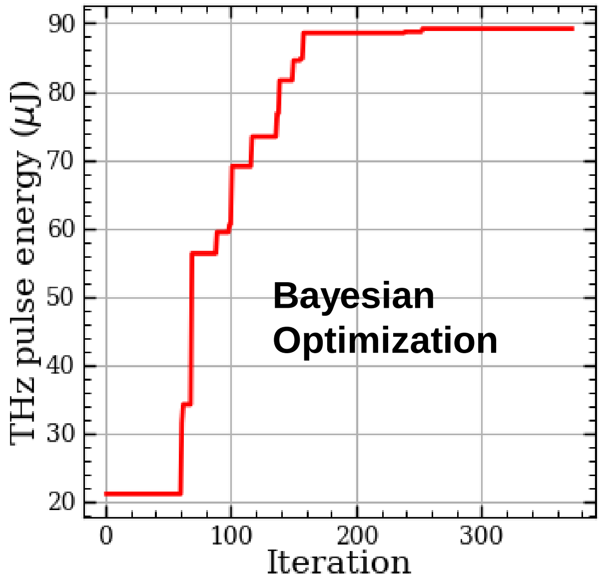
- Lines are from simulation (Astra and Ocelot)
- Markers are from measurements

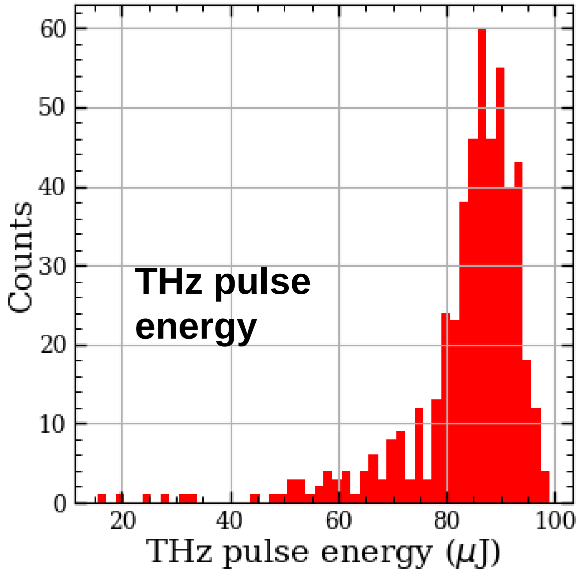




Improving radiation output

- We use a **Bayesian optimizer** (Matlab) to optimize the beam trajectory and phase spaces
  - Two pairs of steering coils → trajectory
  - Long coils along the undulator → trajectory
  - Four to six quadrupole magnets → transverse phase space
  - Booster phase → longitudinal phase space





THz FEL simulations

Shot noise in FEL simulations

- The **shot noise**, which arises from the stochastic nature of the electrons in a bunch, is one of the most critical parameters in the initiation of electron distributions in free-electron lasers (FEL) simulations
- For any distribution of electron bunch or bunch slide, the shot noise can be described by

$$\langle e^{-i\theta_j} \rangle = \frac{1}{n_e} \sum_{j=1}^{n_e} e^{-ikz_j}$$

where n_e is number of electrons in the slice.

- For a **random distribution**, the absolute square of $\langle e^{-i\theta_j} \rangle$ (known as the **form factor**) follows the **negative exponential distribution** with an expectation of $\mathbf{1/_{n_e}}$

$$\left|\langle e^{-i\theta_j} \rangle\right|^2 \sim \mathbb{E}\left(\left|\langle e^{-i\theta_j} \rangle\right|^2, \frac{1}{n_e}\right)$$

where $\mathbb{E}(x,\mu) = \frac{1}{\mu} e^{-x/\mu}$, μ is the expectation value.

- In **Genesis1.3**, the shot noise is introduced by **adding mirror particles** to the macro particles
→ number of macro particles much smaller than number of electrons & **random distribution** in the slice

S. Reiche, Nucl. Instrum. Methods Phys. Res., Sect. A 429, 243 (1999)

Impact of local bunching factors

As found from the standard output of Genesis1.3

- What if the distribution is not random within the range of the resonant wavelength?
→ **Coherent spontaneous radiation**: e.g., from rising slope of flattop or Gaussian profiles

- Consider **"local"** bunching factor: $b_s(z_s) = \frac{\int_{z_s-\lambda/2}^{z_s+\lambda/2} f(z)e^{-ikz}dz}{\int_{z_s-\lambda/2}^{z_s+\lambda/2} f(z)dz}$, z_s is the slice center, $f(z)$ is the distribution of current profile

- For a Gaussian profile, $f(z) = \frac{1}{\sqrt{2\pi}\sigma_z} e^{-\frac{z^2}{2\sigma_z^2}} \cong f(z_s) + (z - z_s)f'(z_s)$, we have

$$b_s(z_s) \cong \frac{z_s}{k\sigma_z^2}\big(\sin(kz_s) - i\cos(kz_s)\big)$$

$$\left|b_{s(z_s)}\right| = \frac{z_s}{k\sigma_z^2}$$

$$\phi_s(z_s) = \tan^{-1}\big(\cot(\mathrm{k}z_s)\big)$$

Impact of local bunching factors

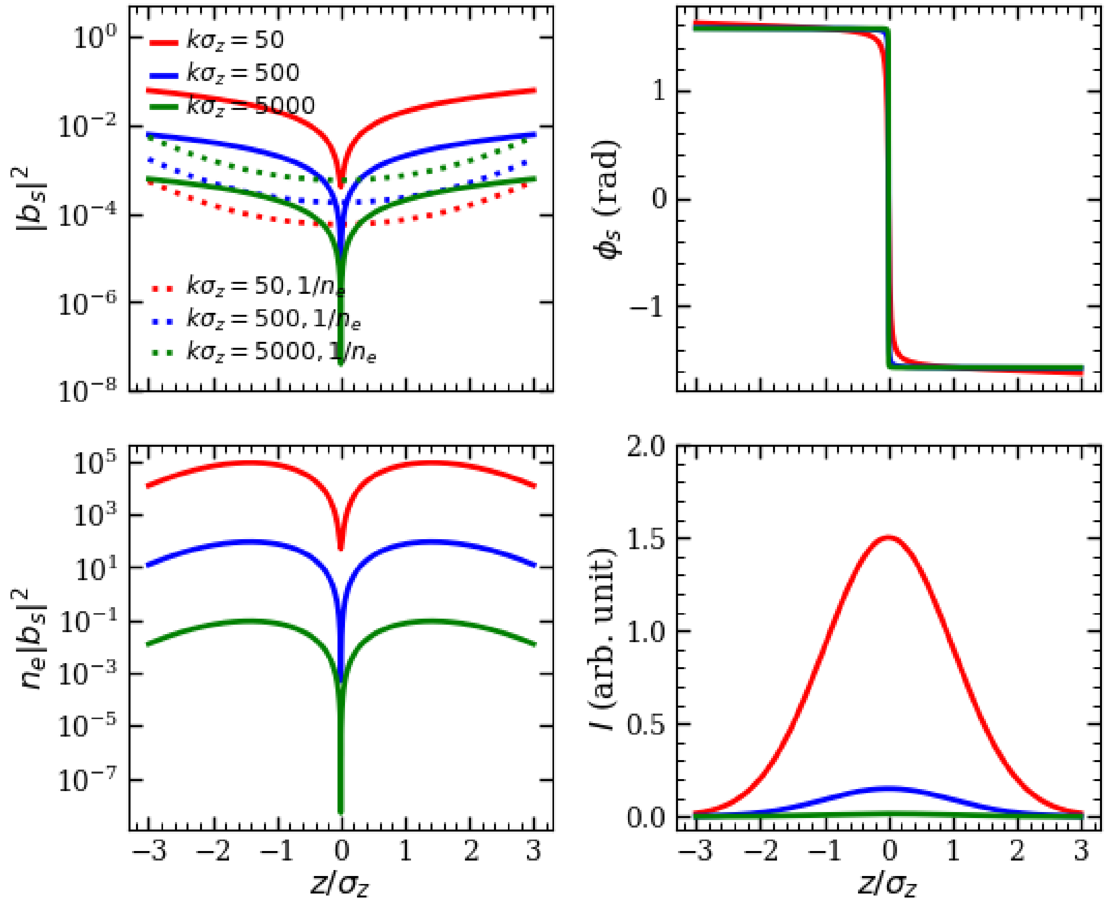
- The radiation from one slice consists of the spontaneous radiation ($\propto n_e$) and the coherent part ($\propto n_e^2|b_s|^2$), their ratio is $n_e|b_s|^2$
  → $n_e|b_s|^2$ is peaked at $z_s = \pm\sqrt{2}\sigma_z$
  → $n_e|b_s|^2 < 1$, spontaneous emission dominates
  → $n_e|b_s|^2 > 1$, coherent emission dominates

- $n_e|b_s|^2 > 1 \Rightarrow \boldsymbol{k^3\sigma_z^3} < \frac{Q}{q_e}(8\pi)^{\frac{1}{2}}e^{-1} \xrightarrow{\text{1 nC}} \boldsymbol{k\sigma_z < 2258}$

- Short-wavelength FEL (1 nC, 1 kA, 1 nm)
  → $k\sigma_z \sim 10^5$, $n_e|b_s|^2 \sim 10^{-8}$

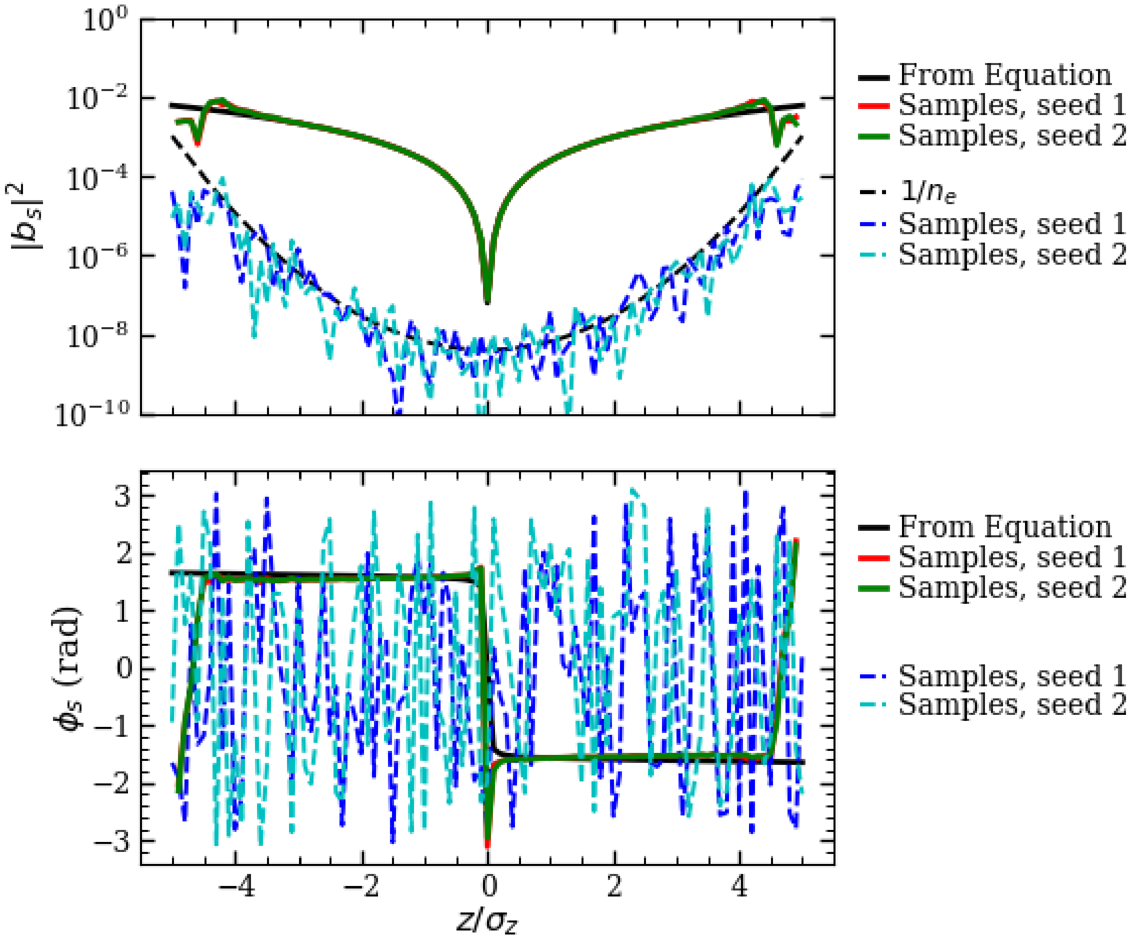
- THz FEL (1 nC, 100 A, 3 THz)
  → $k\sigma_z = 75$, $n_e|b_s|^2 = 27000$

1 nC



Initialization of beam for Genesis1.3

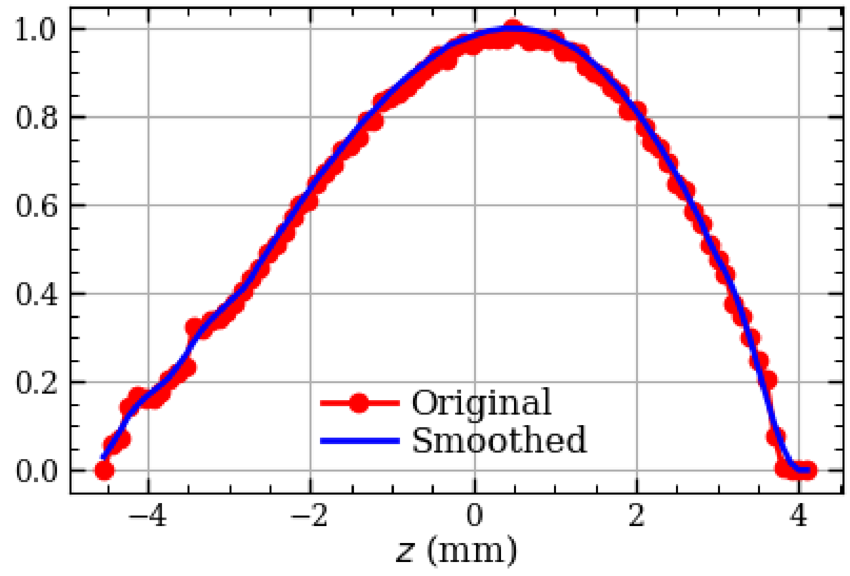
- For each slice, generate samples of **random distribution**, $x_j \sim U(0,1)$, and apply **shot noise** [1]
- Convert the **random** distribution to the **actual** distribution
  e.g, for Gaussian distribution,
  $$z_j \rightarrow \mathrm{F}^{-1}(r_j) = \mu + \sigma\sqrt{2}\mathrm{erf}^{-1}(2r_j - 1)$$
  where F^{-1} is the **inverse CDF** function, μ and σ are mean and standard deviation of the Gaussian distribution
- The local bunching amplitude can be orders of magnitude higher; the bunching phase is also stable

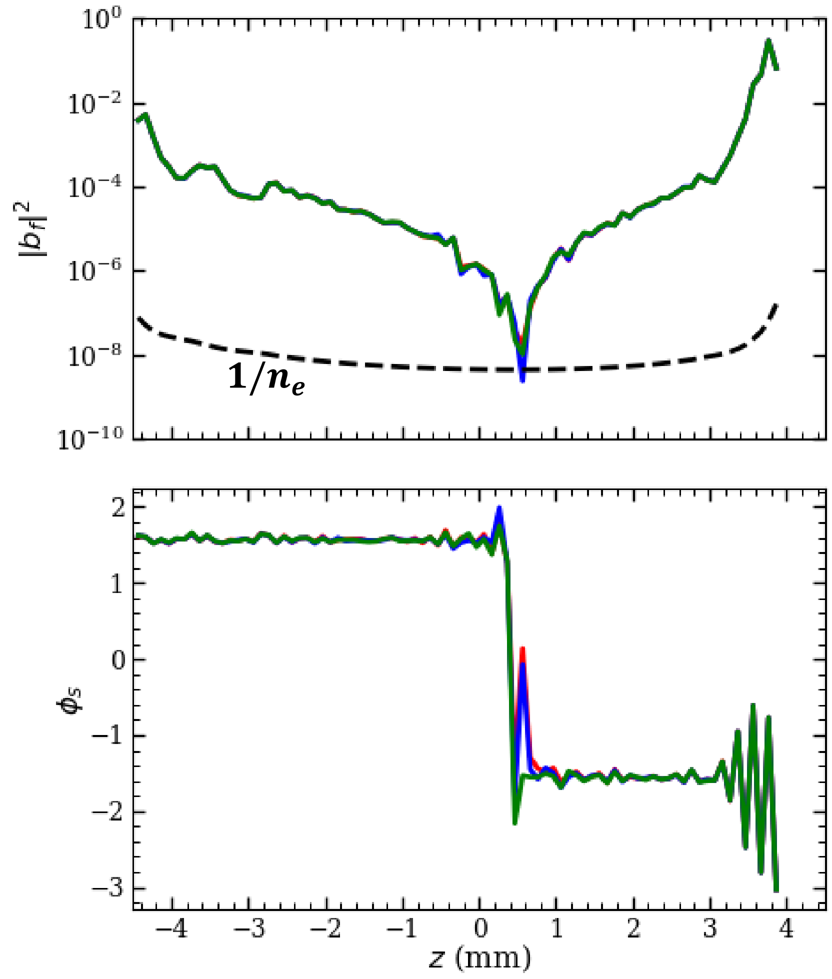


[1] C. Penman and B. McNeil, Optics Communications 90, 82 (1992)

Initialization of beam for Genesis1.3

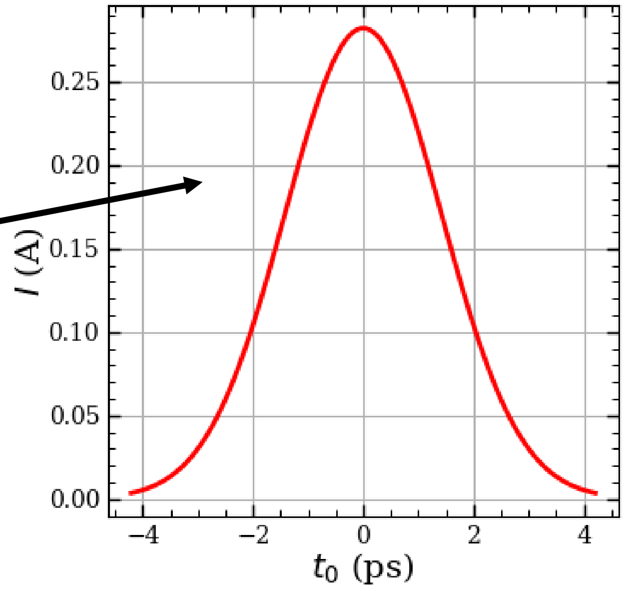
- For any particle distribution obtained from **start-to-end simulation**, we **smooth the current profile** and calculate the **CDF numerically**

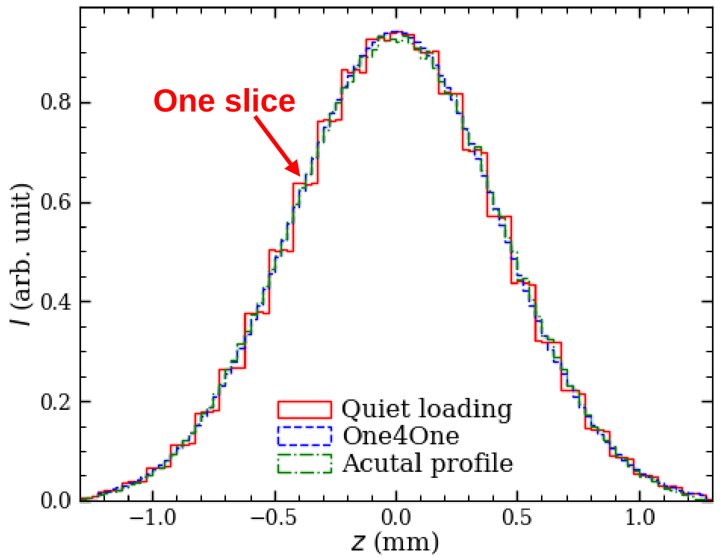




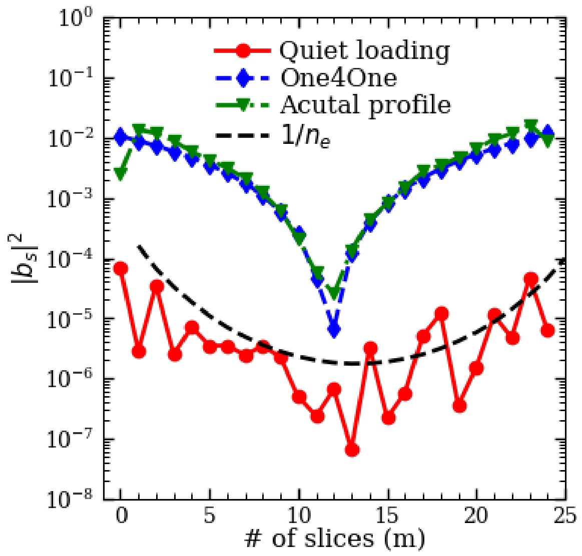
Benchmark simulation

- Electron beam: 17 MeV/c ($\lambda_s = 100\ \mu m$), **1 pC, 0.3 A**
  - One4one = **False**, quiet loading, Nm = 26*32768 = **851,968**
  - One4one = **True**, **Ne = 6,241,509**
  - One4one = **False**, smoothed profile, Nm = 26*32768 = **851,968**

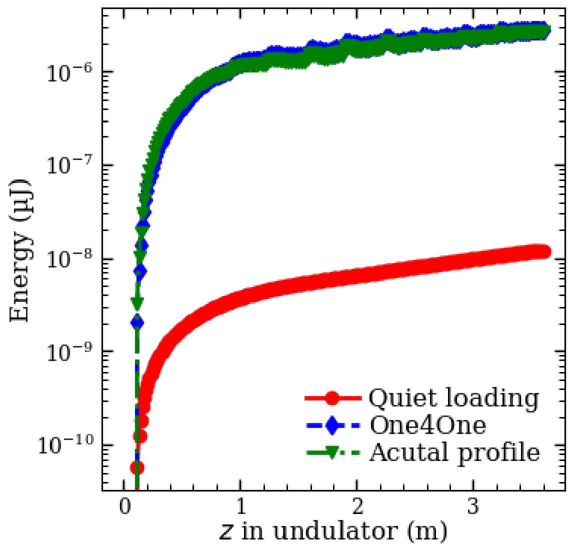




Current profile in Genesis4



Initial bunching in Genesis4



Gain curves from Genesis4

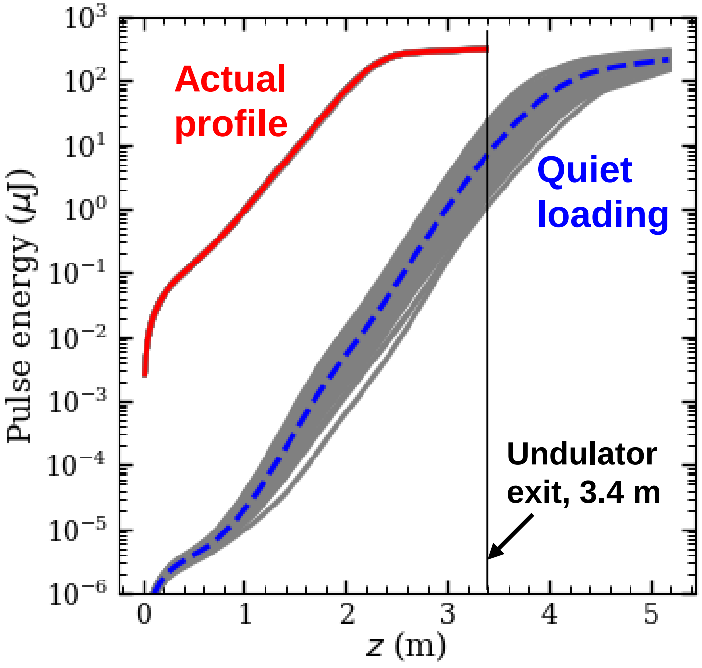
Using input from start-to-end simulation

TABLE II. Comparison of THz pusle properties.

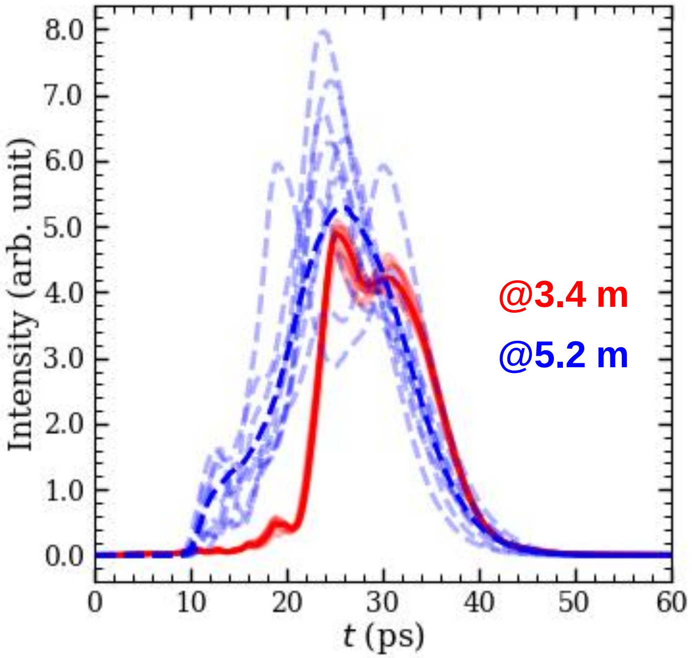
Parameters	case I	case II	Units
Current profile in slice	actual	random	
Peak power	923.77 ± 6.87	644.24 ± 98.66	MW
Pulse energy	308.14 ± 2.29	214.89 ± 32.91	µJ
Center wavelength	98.88 ± 0.09	100.76 ± 0.59	µm
Spectral width	1.95 ± 0.08	2.47 ± 0.49	µm
Pulse duration	5.38 ± 0.04	6.21 ± 0.70	ps
Arrival time jitter	0.10	1.30	ps

- Electron beam: 17 MeV/c ($\lambda_s = 100\ \mu\text{m}$), **2 nC, 112 A**
  - One4one = **False**, smoothed profile, Nm = 85*32768
  - One4one = **False**, quiet loading, Nm = 85*32768

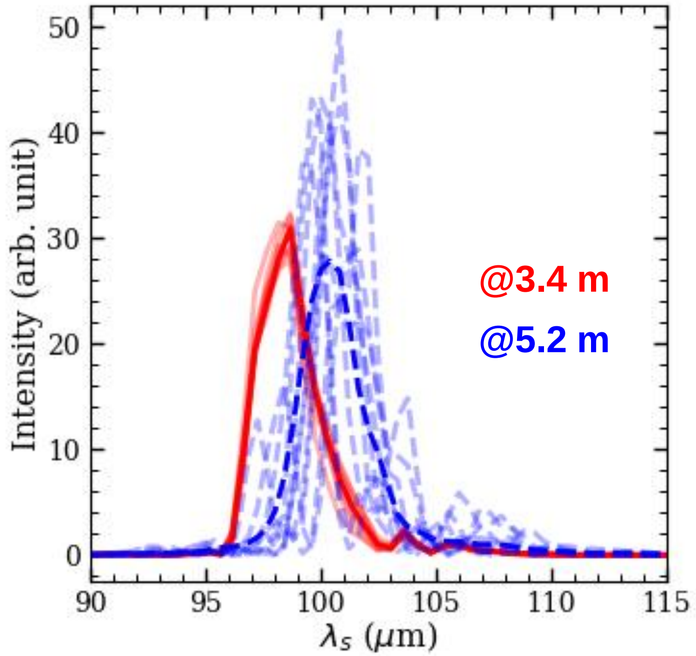
Gain curves



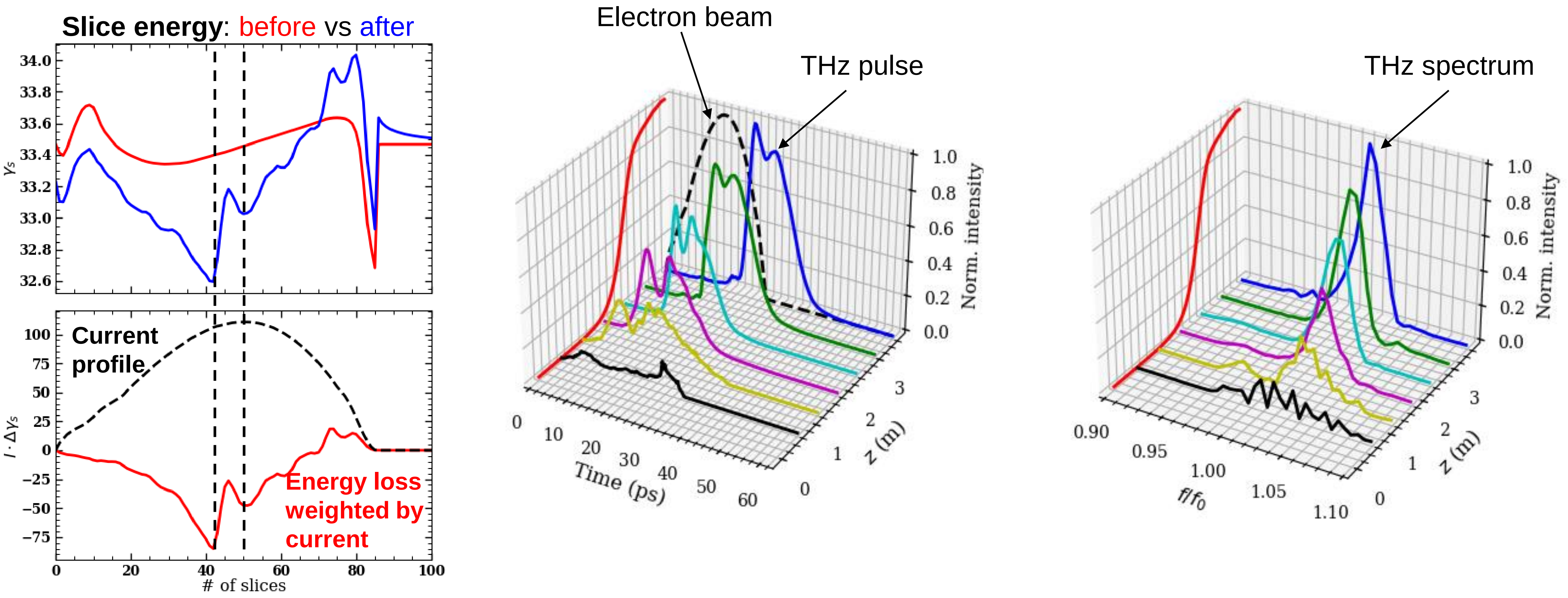
Temporal profiles



Spectrum



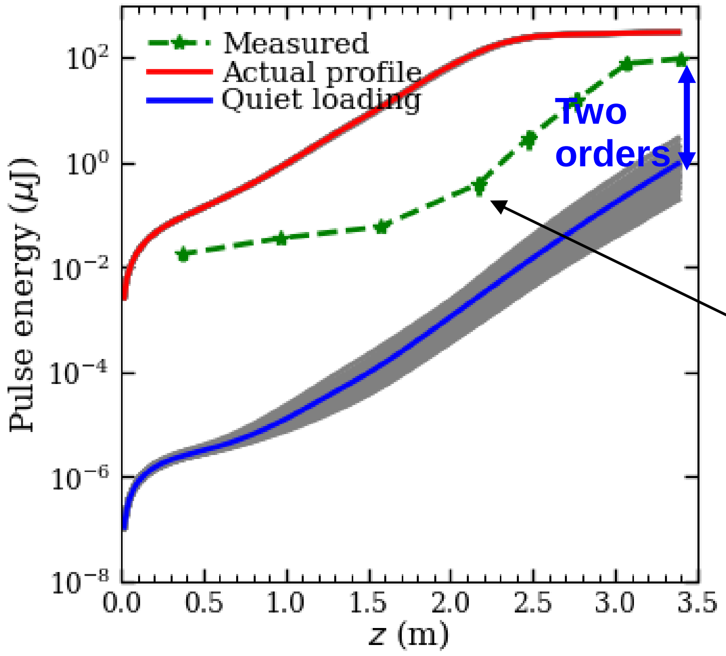
Using input from start-to-end simulation



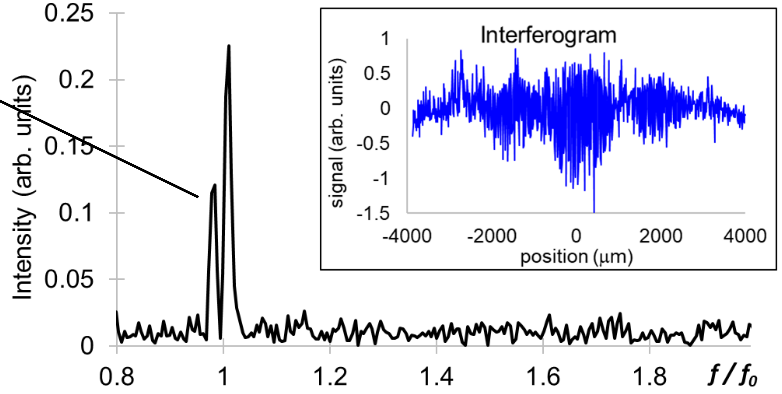
M. Krasilnikov, *et al.*, Phys. Rev. Accel. Beams., 28(3):030701, 2025

Comparison with experimental data

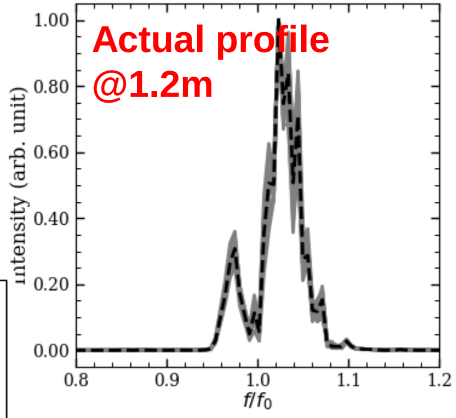
- The measured pulse energy was about **40-50 μJ for 2 nC**; considering transmission loss of 50%, about **100 μJ has been generated**
- From simulations, we got **300-500 μJ with the actual profile (**but only **several μJ with quiet loading)**
  Possible reasons: beam trajectory (due to undulator transverse gradient + EMF), wakefields (geometric and resistive wall), waveguide effect, etc

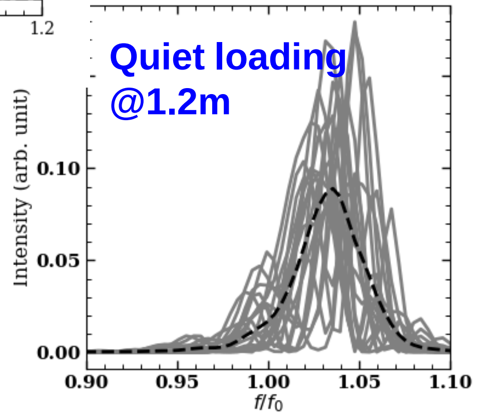


- Spectrum from measurement and simulations



Measured with FTIR (E. Zapolnova)





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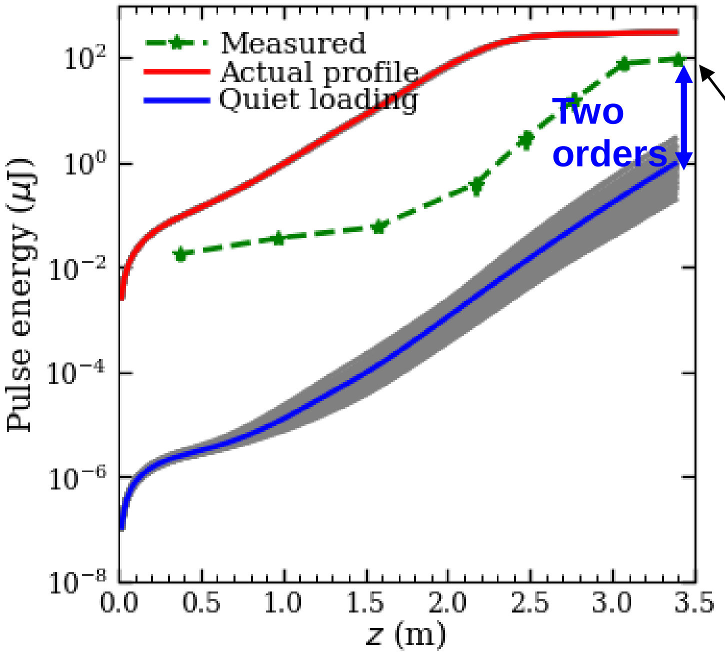
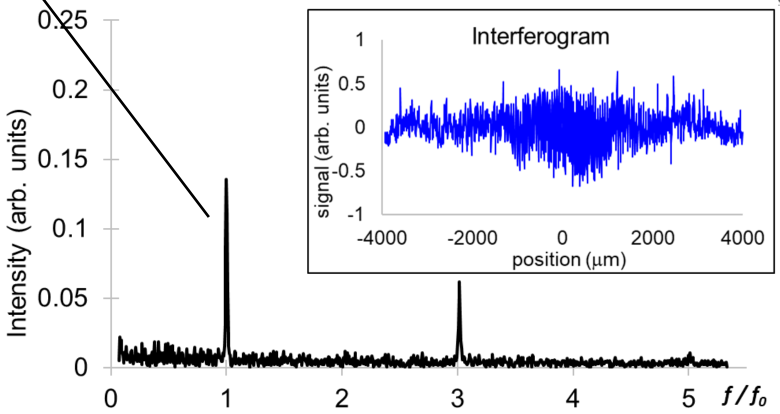


- Spectrum from measurement and simulations



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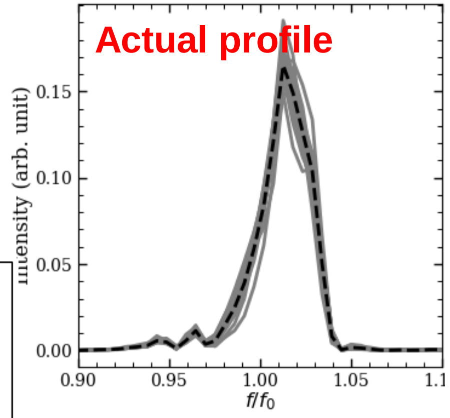
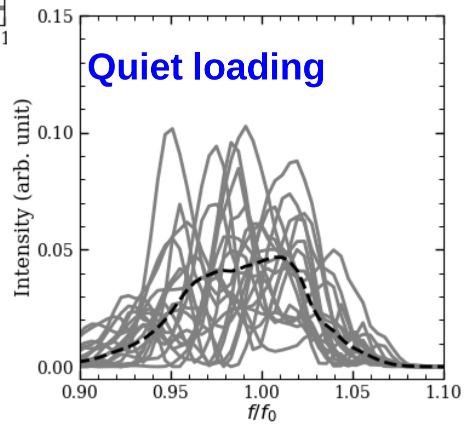
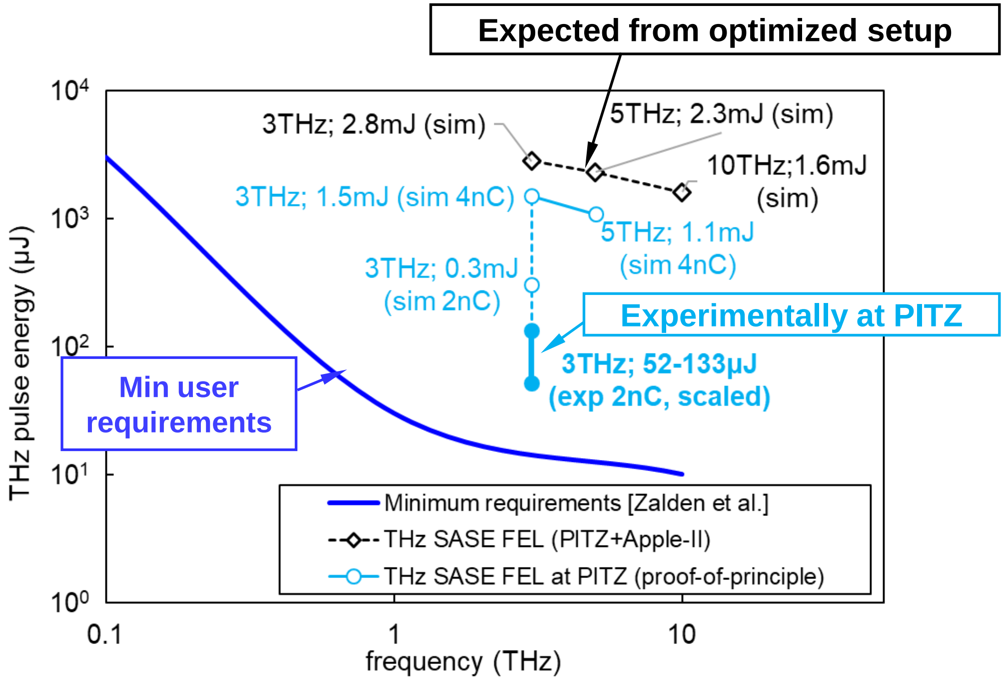




Summary

- The THz FEL at PITZ: **first lasing in 2022**, currently generating **>100 μJ single pulse energy at 3 THz**
  Routine tuning: Beam transport and matching + Bayesian optimization of last magnets

- The THz FEL starts from **coherent spontaneous radiation**, which comes from the rising slope of the electron beam current profile
  → lower requirement on peak current + better stability



- **R&D on THz FEL** continues at PITZ:
  1) Developing or testing THz diagnostic techniques, e.g., EOS
  2) Understanding and modeling of THz FEL and
  3) Improving performance by laser shaping, bunch compression, seeding, etc

THz@PITZ Team and Collaboration

Proof-of-principle experiment on high power THz source

DESY Zeuthen

Physicists:
- Z. Aboulbanine*
- G. Adhikari*
- *N. Aftab*
- *P. Boonpornprasert**
- *G. Georgiev**
- J. Good
- M. Gross
- A. Hoffmann
- E. Kongmon*
- *M. Krasilnikov*
- *B. Li*
- *X.-K. Li*
- *A. Lueangaramwong**
- R. Niemczyk*
- A. Oppelt
- H. Qian*
- C. Richard
- F. Stephan
- G. Vashchenko
- T. *Weilbach**
- *D. Xu*
- *X. Zhang**

* → left PITZ for other lab

Special thanks to CANDLE colleagues participated in THz commissioning and lasing shifts!

Engineers and Technicians:
- R. General
- L. Heuchling
- M. Homann
- L. Jachmann,
- D. Kalantaryan
- W. Köhler
- G. Koss
- S. Maschmann
- D. Melkumyan
- F. Müller
- R. Netzel
- B. Petrosyan
- S. Philipp
- M. Pohl
- C. Rüger
- A. Sandmann-Lemm
- M. Schade
- E. Schmal
- J. Schultze
- S. Weisse

SLAC
- A. Brachmann
- N. Holtkamp
- H.-D. Nuhn

DESY Hamburg
- E. Schneidmiller
- M. Yurkov
- B. Krause
- M. Tischer
- P. Vagin

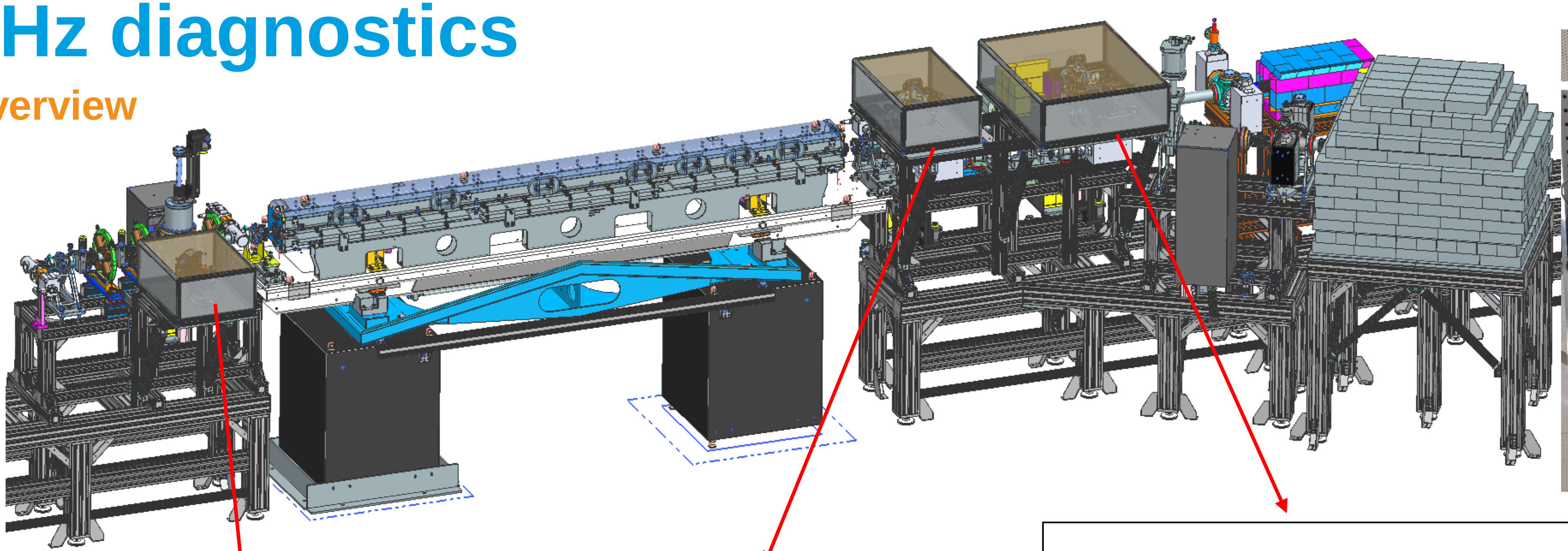
Uni Hamburg
- J. Rossbach
- W. Hillert

Thank you!

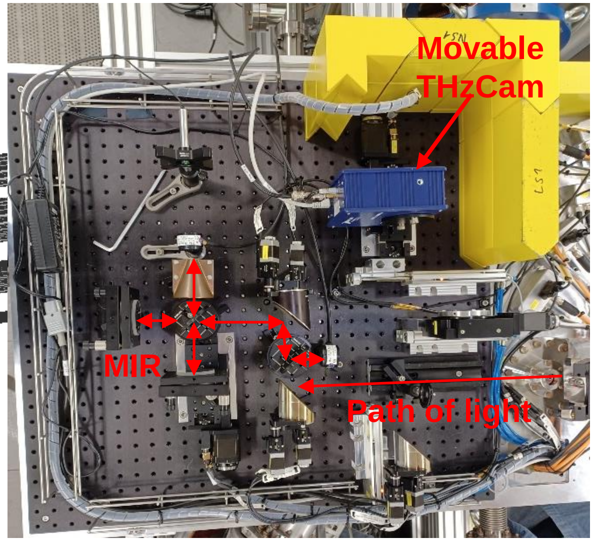
Backup

THz diagnostics

Overview



Current TD3 layout



CTR/TD1:

- **Quartz** vacuum window
- ~0.2 m transport in vacuum, ~0.5 m transport in air
- Focusing by using 90° off-axis ellipsoidal and parabolic mirrors

- Pulse energy ← pyroelectric detector
- THz spectrum ← Michelson interferometer

TD2:

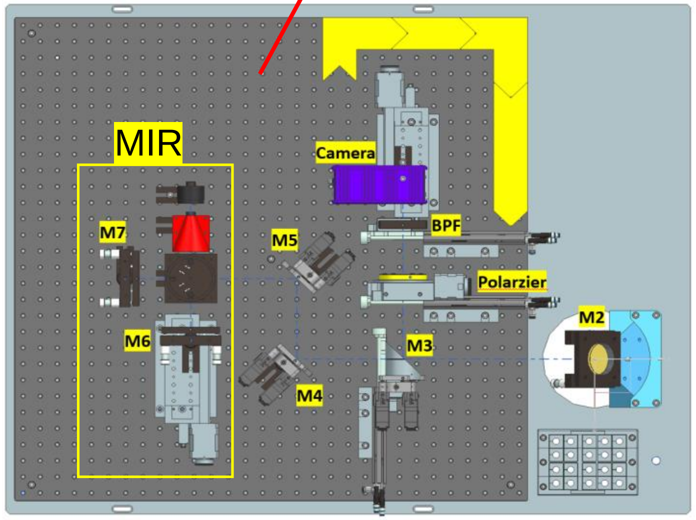
- ~0.5 m transport in vacuum, ~0.5 m transport in air
- **Diamond** vacuum window
- Focusing by using 90° off-axis ellipsoidal mirror

- Pulse energy ← pyroelectric detector
- Single-shot EOS?

TD3:

- ~1.5 m transport in vacuum, 1-1.5 m transport in air
- **Diamond** vacuum window
- Focusing by using 90° off-axis ellipsoidal and parabolic mirrors

- **Pulse energy ← pyroelectric detectors**
- **Trans. profile ← THz camera**
- **Polarization ← THz polarizer**
- **THz spectrum ← Michelson interferometer**
- **Single-shot EOS?**

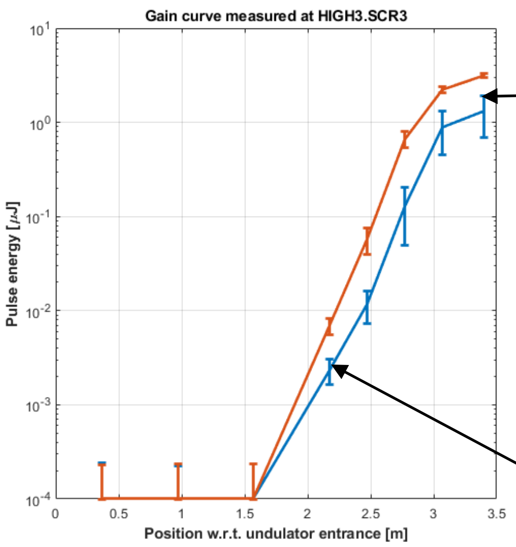


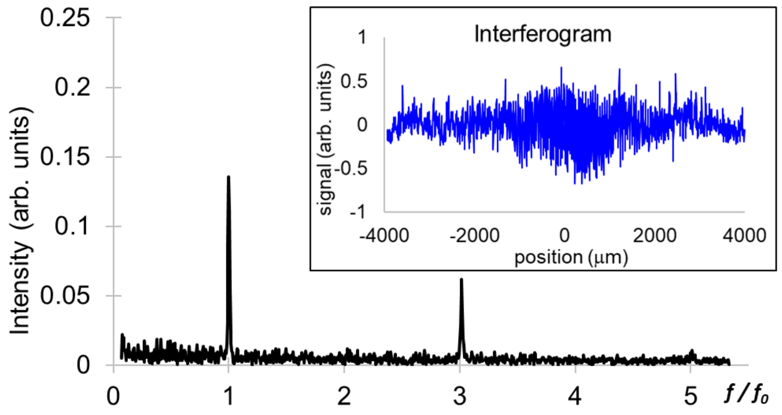
Available; Planned/ongoing (short term); Wished (long term)

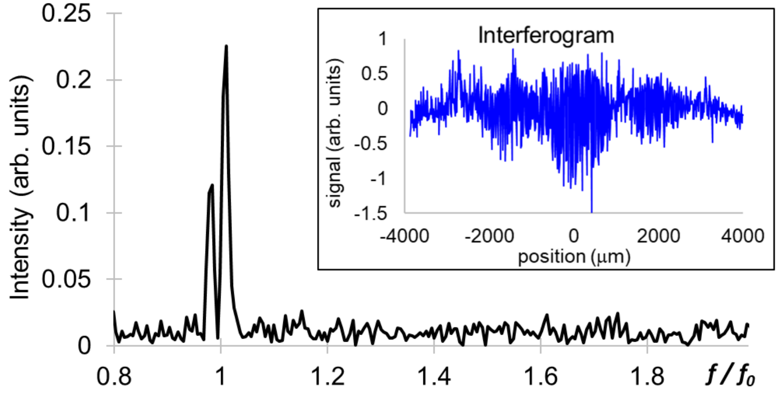
Spectrum measurements

Measured with the FTIR spectrometer from FLASH (E. Zapolnova, THz beamline at FLASH, waiv.ai)

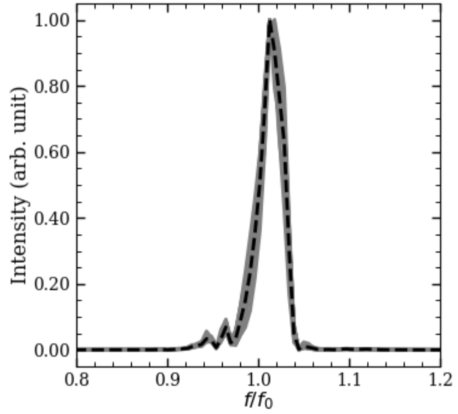
- 2 nC beam, central frequency ~2.82 THz ($\lambda_{\mathrm{rad}} = 106.5$ μm), reference signal from PITZ pyro

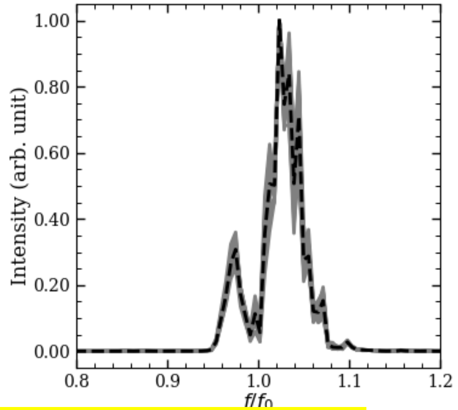






vs GENESYS1.3 simulations



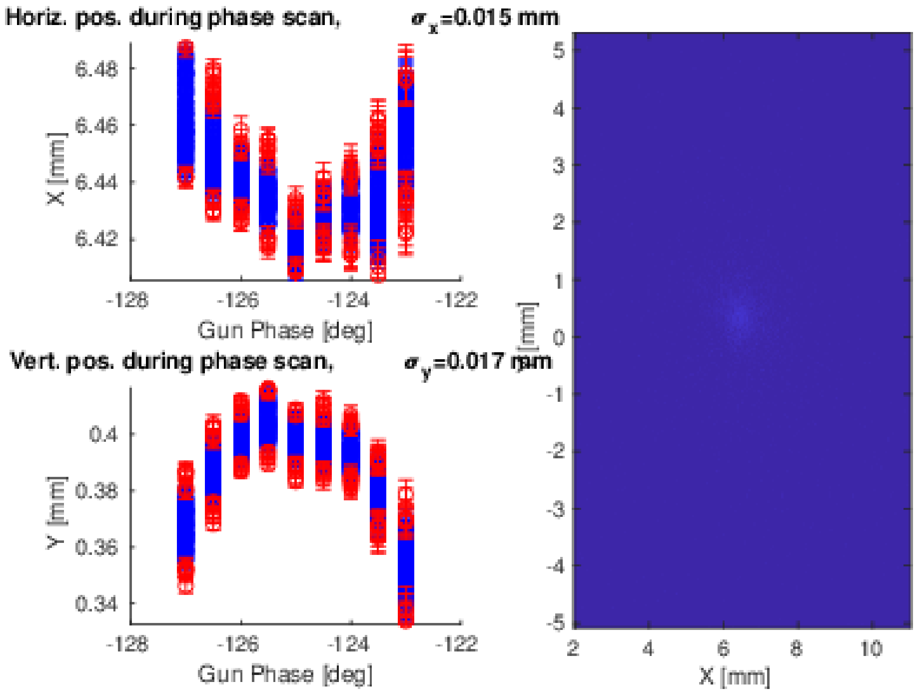


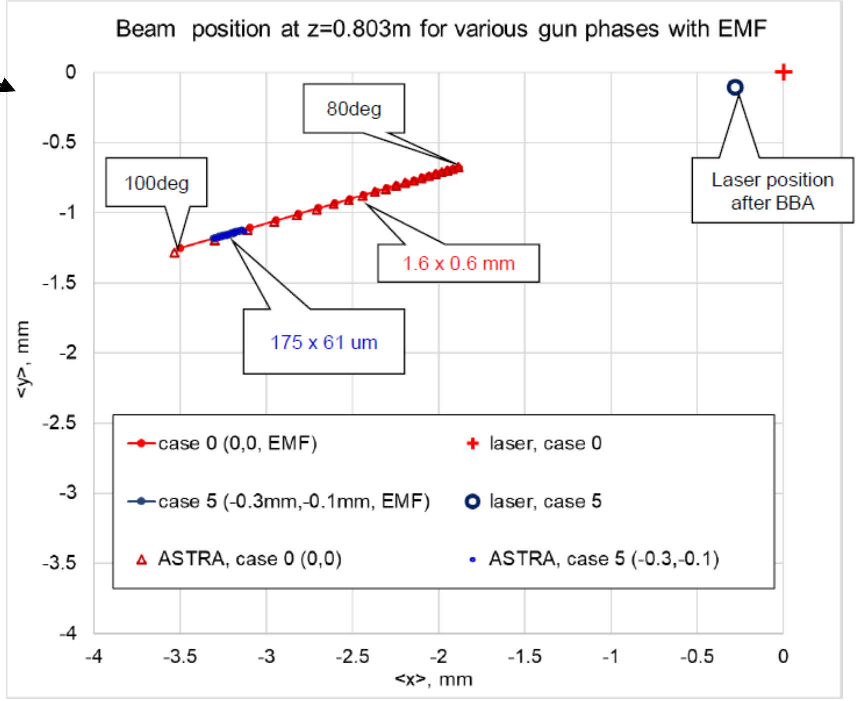
- **Narrow bandwidth**
- **High harmonics (3rd and signature of 5th)**
- **Spectrum shape in linear regime**

Optimization of photoinjector

Beam based alignment (BBA)

- Routine procedures before emittance optimization
  - **Laser BBA:** Align the beam with the RF field axis in the gun: $\Delta r = 0$
    Idea: RF field is rotationally symmetric, RF kick ~ $\Delta r \cdot \Delta\phi$
    Issue: Earth magnetic field (**EMF**) → (-0.3, -0.1) um instead of (0, 0) at the center





M. Krasilnikov, PPS talk, 2022-03-31

From K. Peetermans, DESY summer school 2022 report

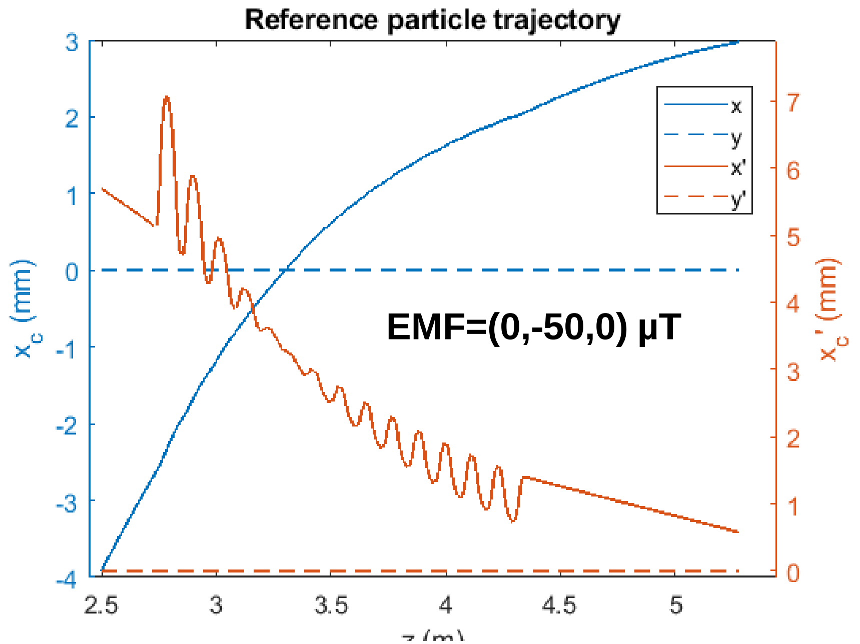
Optimization of photoinjector

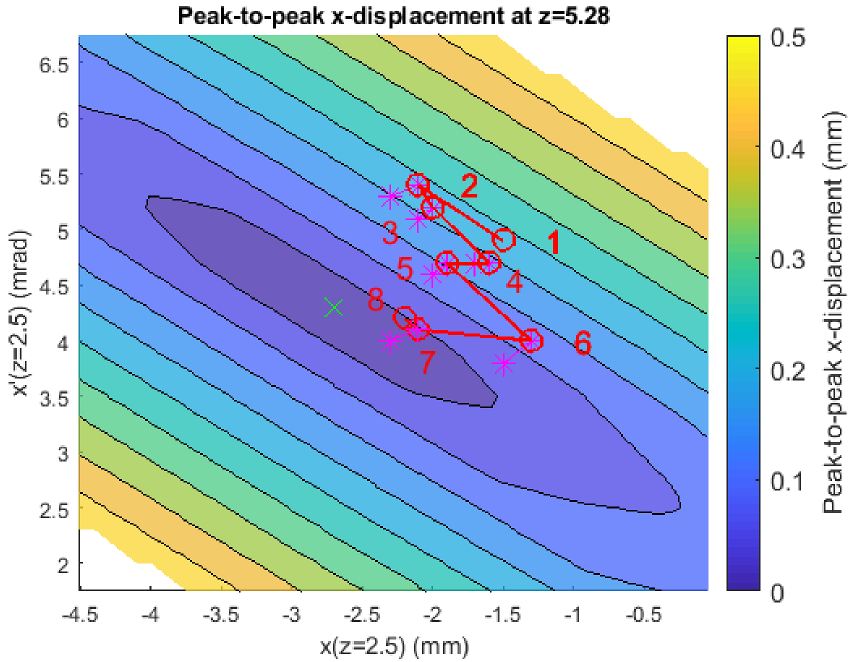
Beam based alignment (BBA)

- Routine procedures before emittance optimization
  - **Booster BBA**: Align the beam with the RF field axis in the booster; also not perfect due to the existence of EMF
    → The beam is offset by ~3 mm with an angle ~1 mrad after booster
    → Prediction & correction with the data from simulations, seems to work

- Ultimate solution to EMF: **Helmholtz coil?**

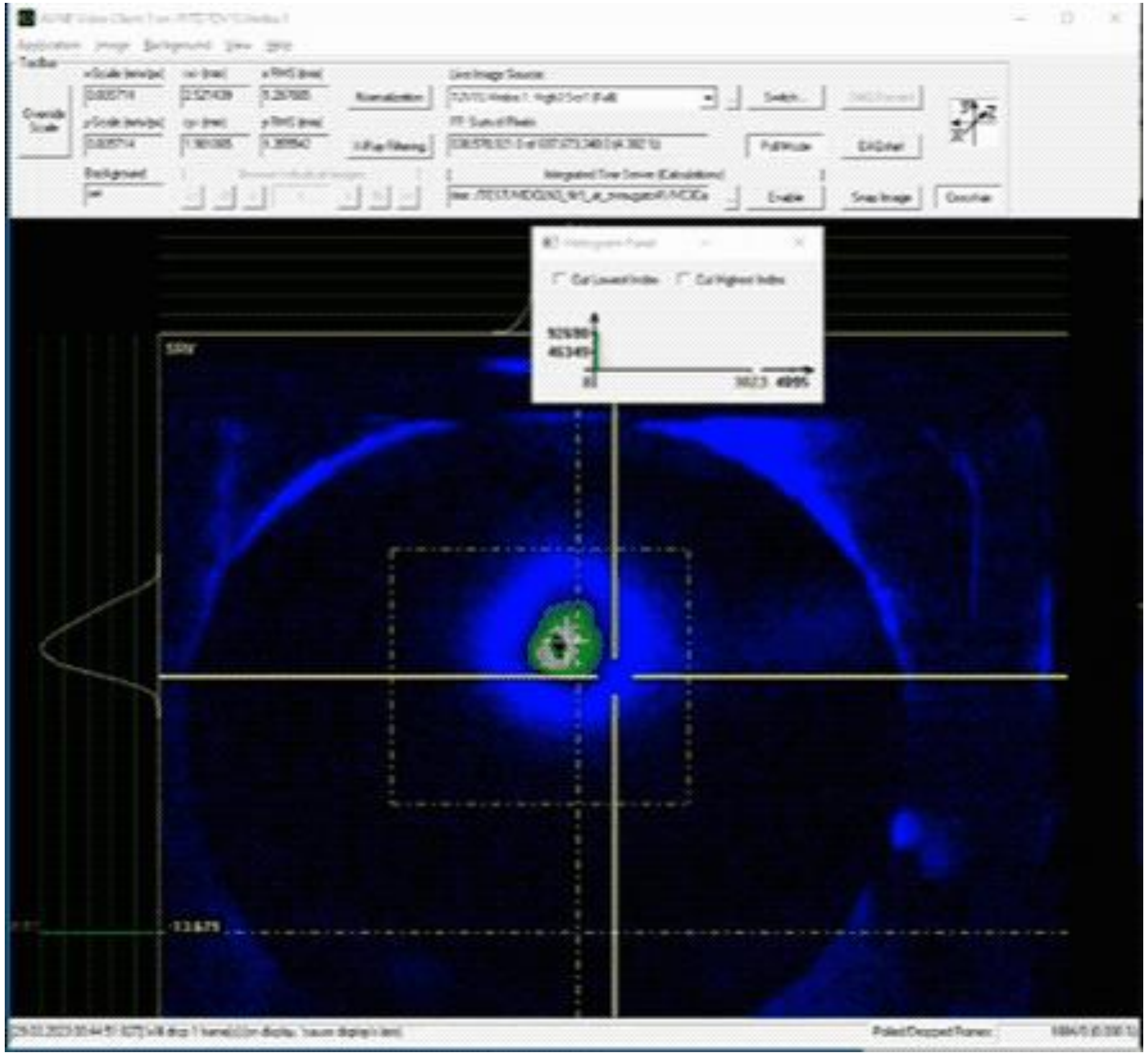
- Other procedures
  - Solenoid BBA, usually done after installation
  - Gun quads optimizer → compensate the asymmetric distribution of laser and/or the quadrupole component of the solenoid fields; currently done with Simplex method





Why trajectory matters?

e^- beam at High3.Scr1
(in front of the undulator)
changed with upstream
steerers



Guess: dispersion effects?
Solution: Minimize the use of
steerers and make quadrupoles
steering free

Quad steering free beam transport

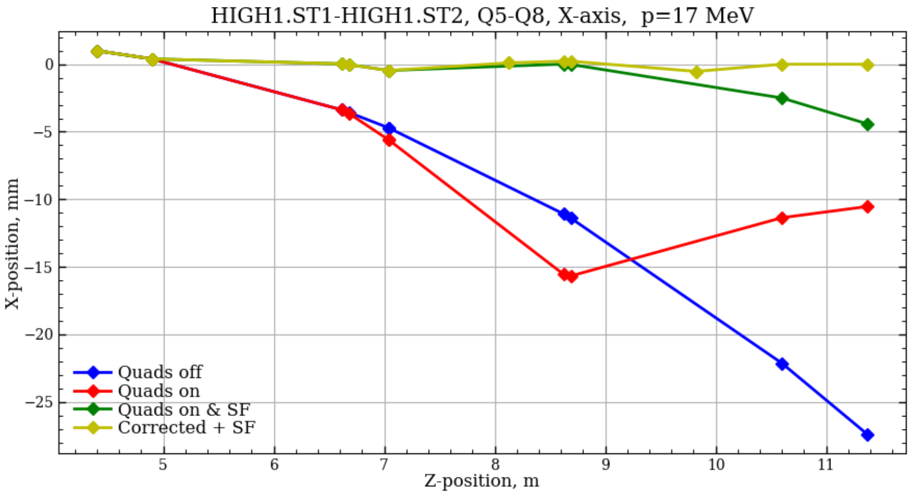
Simulations by D. Dmytriiev

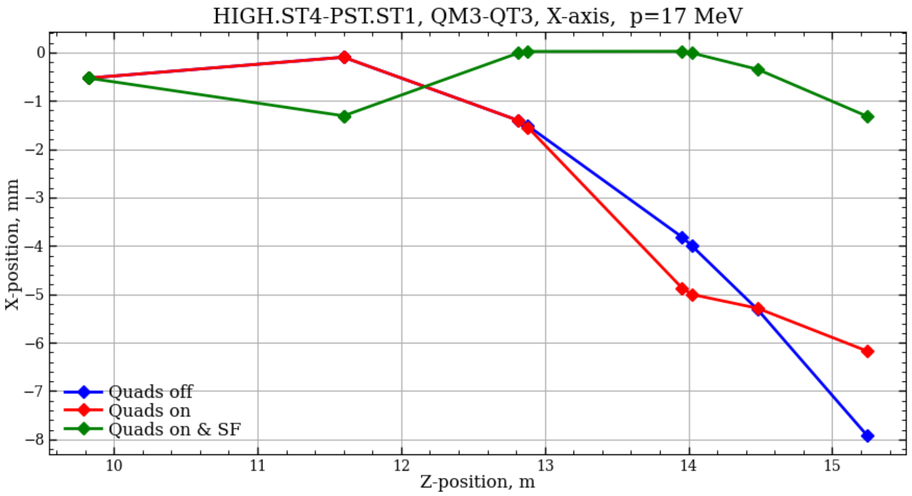
- Idea
  - Response matrices with and without quads are **different**
  - When all quads are made steering free
    → trajectories with and without quads will be **same**
  - By measuring the difference, the trajectory inside the quads can be set to beam axis by tuning steerers with

$$\boldsymbol{\Delta\theta} = -(\boldsymbol{H_1} - \boldsymbol{H_0})^{-1}(\boldsymbol{x_1} - \boldsymbol{x_0})$$

where H_0 and H_1 are response matrices w/o and w/ quads,
x_0 and x_1 are beam positions measured w/o and with the quads

- Limits
  - Low steerers may need to be tuned in order to make High1 quads steering free (otherwise currents out of limit)
  - No enough steerers to make all relevant quads (especially High2.Q3-Q5) steering free



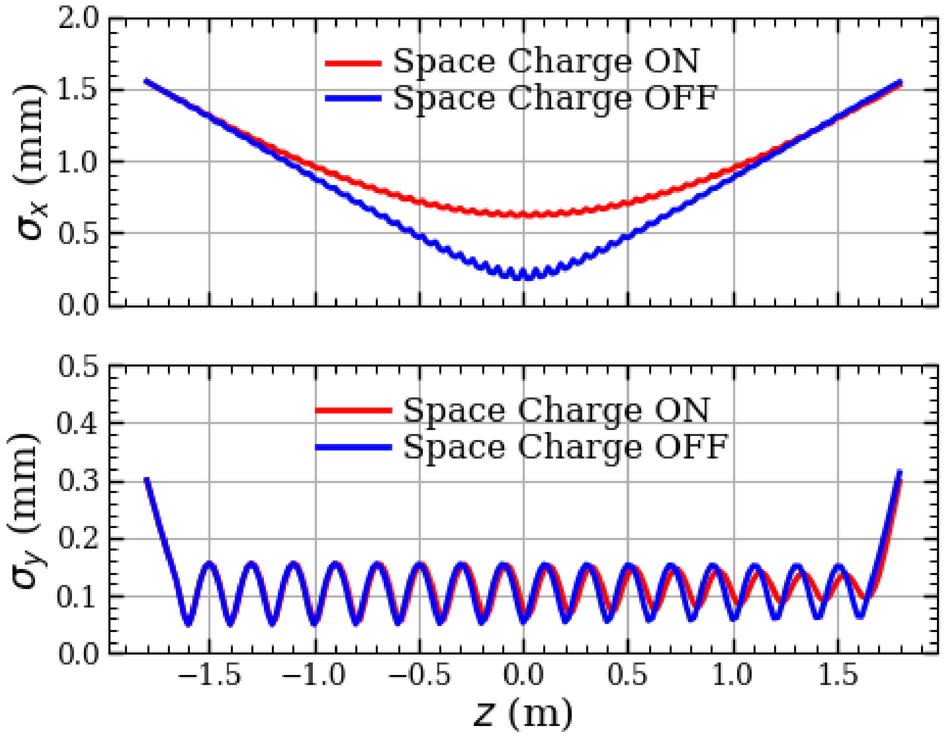


Matching of transverse phase space

For LCLS-I undulator

- The LCLS-I undulator vacuum chamber is very "small" for 17 MeV/c electrons
- Space charge force and magnetic focusing force from the undulator fields can lead to a rapid growth of the beam size and therefore beam loss, if the transverse phase space is not well matched

In the horizontal plane, the motion is dominated by the space charge; in the vertical plane, it is up to the undulator focusing fields
→ Independent parameter scan in two planes

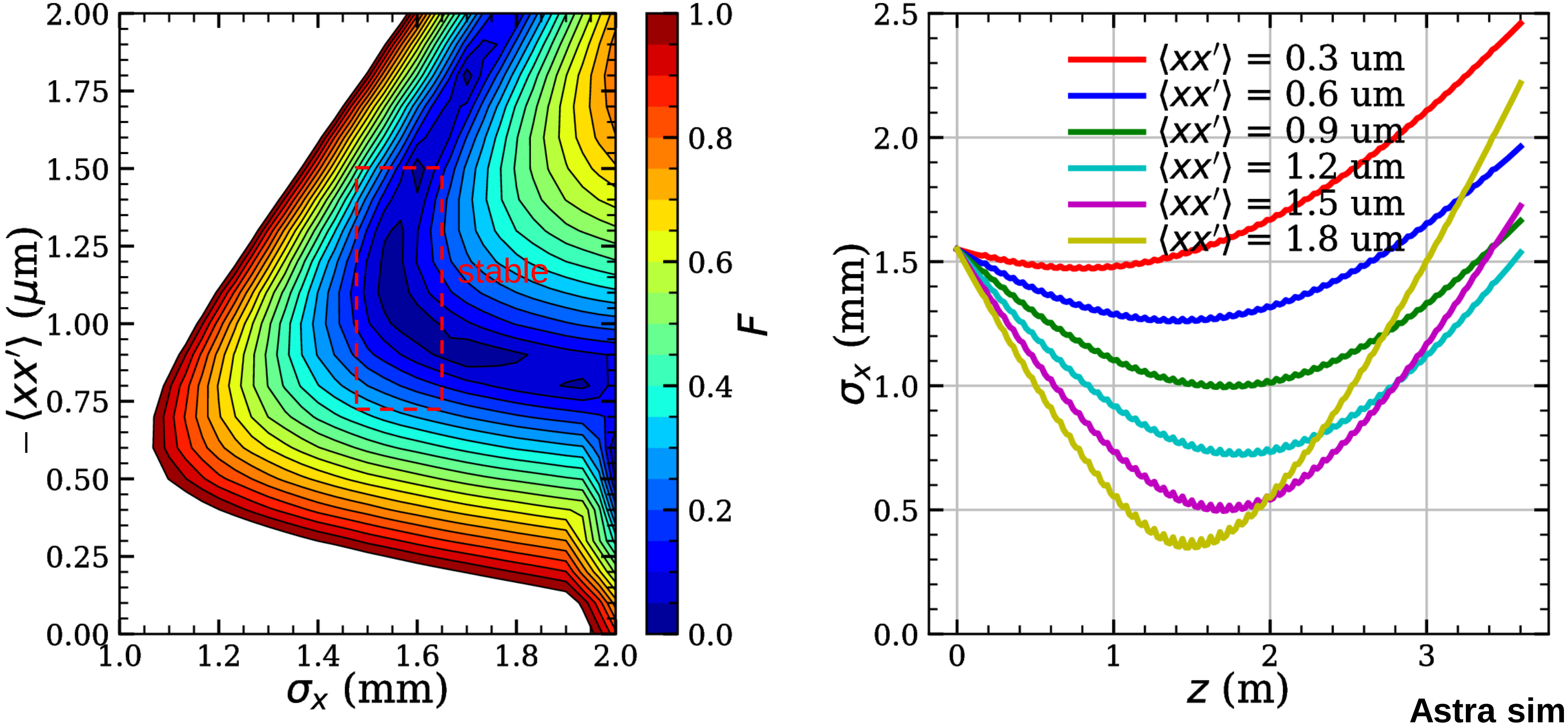


Scan of transverse phase space for matching

In horizontal plane

- For the momentum of 17 MeV/c and normalized emittance of 4 um

$$F = |\sigma_x^{in} - \sigma_x^{out}|$$



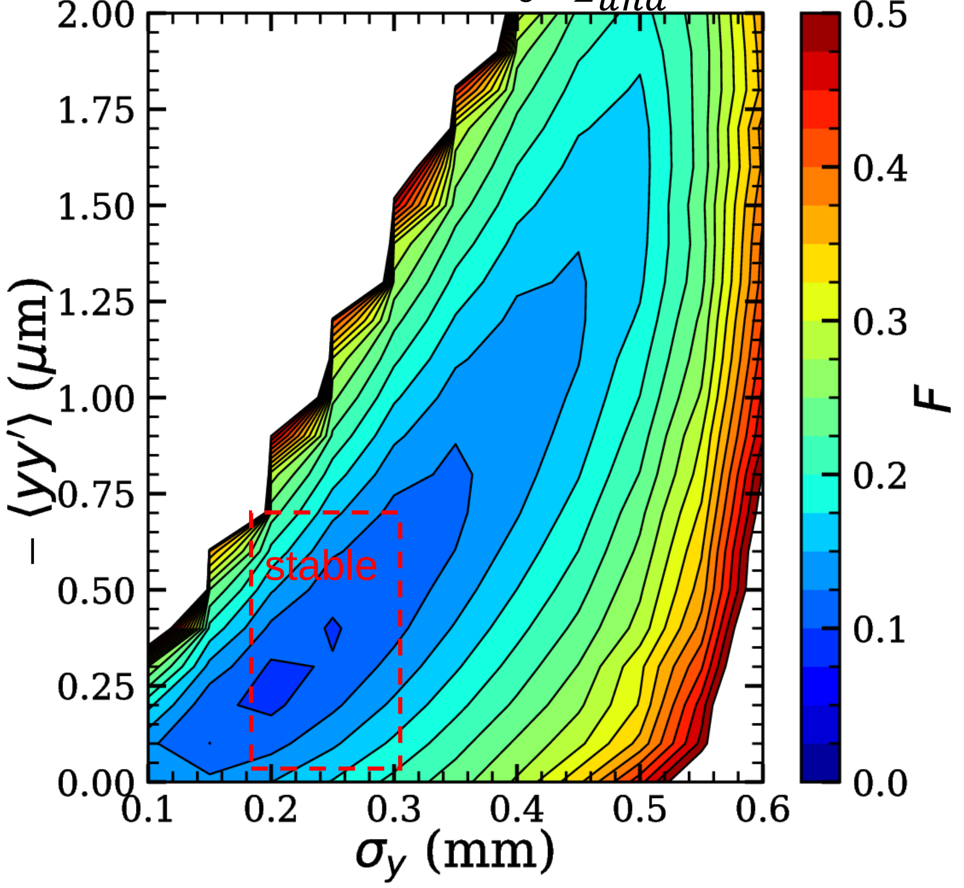
Astra simulations

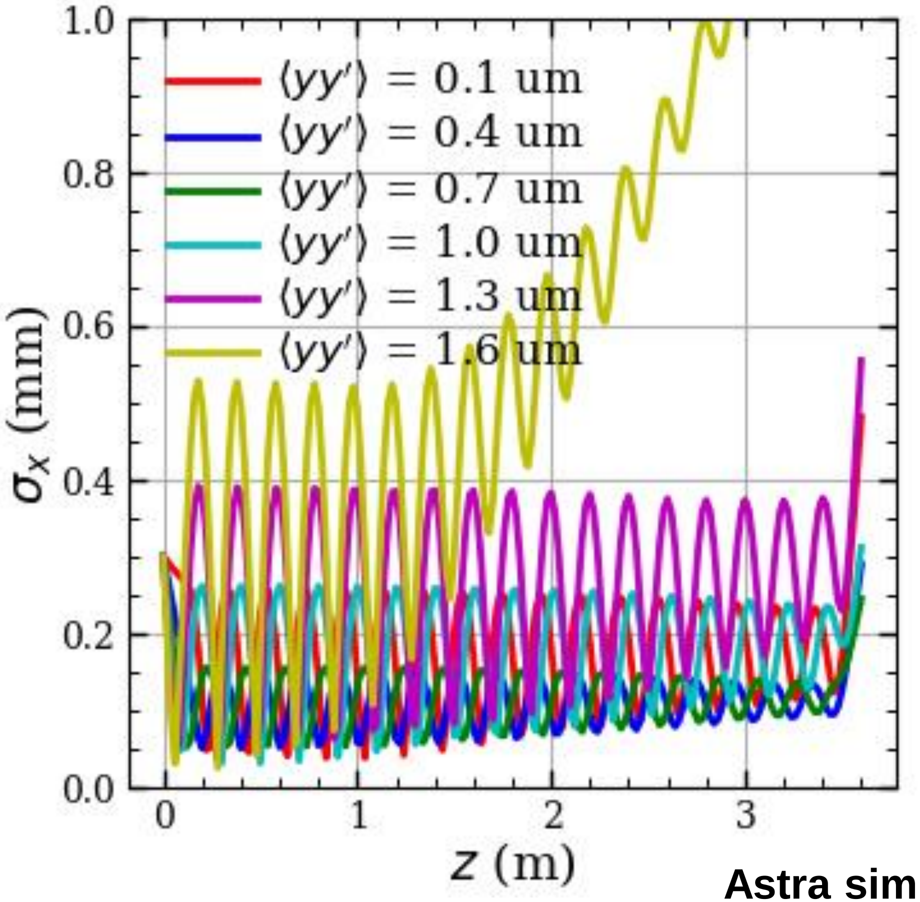
Scan of transverse phase space for matching

In vertical plane

- For the momentum of 17 MeV/c and normalized emittance of 4 um

$$F = \langle \sigma_y \rangle_{0 \to L_{und}}$$





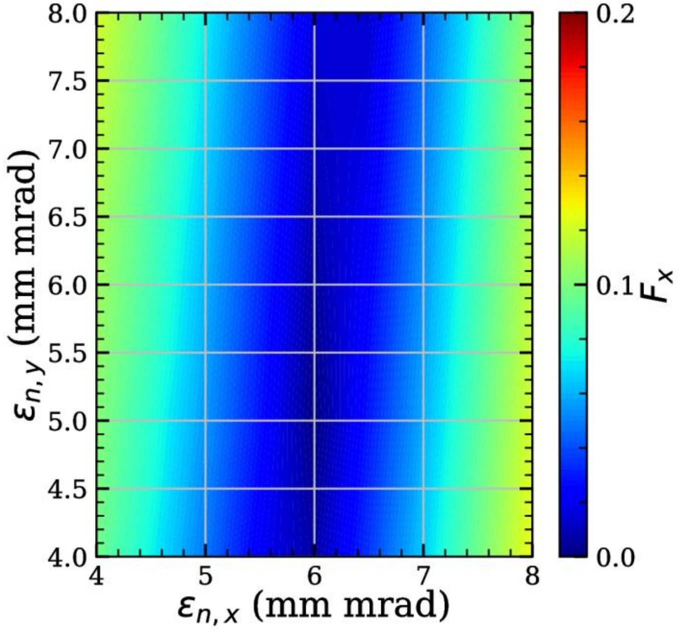
Astra simulations

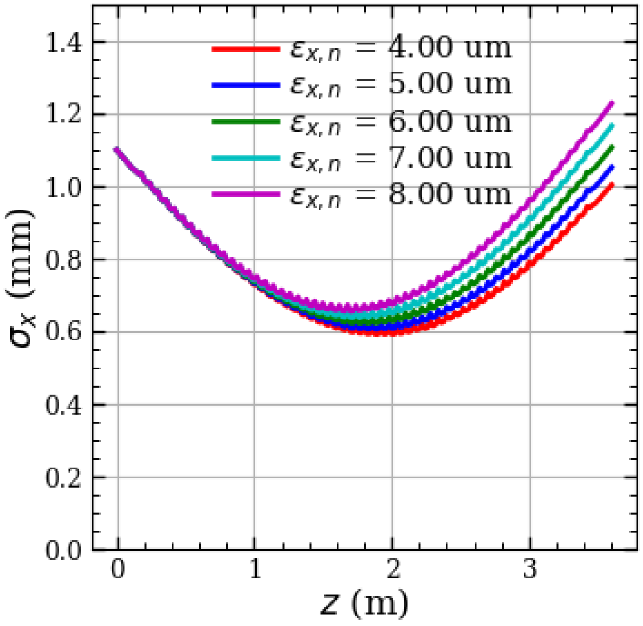
Scan of transverse phase space for matching

Beam emittance scan

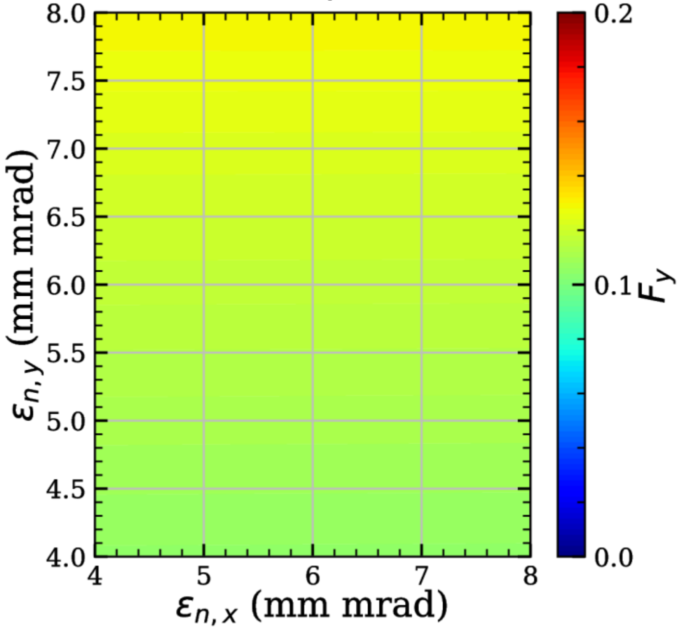
- Here the beam size and covariance are fixed and the x and y emittances are scanned
- The beam envelopes in the undulator are not affected much

For x





For y



Phase space matching (6 parameters) → beam size and covariance (4)

Astra simulations