Overview of Start-to-End Simulation Activities towards CW Regime Operation of XFEL

Kickoff • Oct.-Nov.2020

Ye Chen & Martin Dohlus

On behalf of S2E BD Group at DESY, Virtual BD Meeting, 10.11.2020

Thanks to co-workers: D. Bazyl, I. Zagorodnov, F. Brinker, S. Tomin, S. Meykopff, T. Limberg, W. Decking, B. Beutner, E. Vogel, M. Scholz, M. Guetg, S. Liu, E. Schneidmiller & many others from PITZ, MPY, MXL & MSL

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

DESY.

Outline

- Background, Motivation & Goals
- **SRF-gun based cw injector optimization (D. Bazyl)**
- RF energy gain budgets in CW regime (inputs from E. Vogel)
- Accelerator S2E simulation capabilities (injector → undulator)
  - ✓ OCELOT, IMPACT-Z
- Summary & Outlook
- **Backup Slides**
  - ✓ **SASE simulations**

Background

✓ **R&D activities towards a CW XFEL under continuous reviews of DESY Machine Advisory Committee**

→ Not only about a CW injector

→ But also involving S2E BD studies (Injector to Undulator)

✓ **Forward-looking guidance (2014)**

ELSEVIER

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment

Volume 768, 21 December 2014, Pages 20-25

Prospects for CW and LP operation of the European XFEL in hard X-ray regime

R. Brinkmann, E.A. Schneidmiller, J. Sekutowicz, M.V. Yurkov

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https://doi.org/10.1016/j.nima.2014.09.039

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The European XFEL will operate nominally at 17.5 GeV in SP (short pulse) mode with 0.65 ms long bunch train and 10 Hz repetition rate. A possible upgrade of the linac to CW (continuous wave) or LP (long pulse) modes with a corresponding reduction of electron beam energy is under discussion for many years. Recent successes in the dedicated R&D program allow to forecast a technical feasibility of such an upgrade in the foreseeable future. One of the challenges is to provide sub-Ångström FEL operation in CW and LP modes. In this paper we perform a preliminary analysis of a possible operation of the European XFEL in the hard X-ray regime in CW and LP modes with electron energies of 7 GeV and 10 GeV, respectively. We consider lasing in the baseline XFEL undulator as well as in a new undulator with a reduced period. We show that, with reasonable requirements on electron beam quality, lasing on the fundamental will be possible in the sub-Ångström regime. As an option for generating brilliant photon beams at short wavelengths we also consider harmonic lasing that has recently attracted a significant attention.

Background (cont'd)

✓ **R&D activities regarding choices of the CW gun in light of S2E simulation results**

→ Performance of various CW injectors in S2E beam dynamics

Choice of the gun for CW operation of the European XFEL

Igor Zagorodnov and Martin Dohlus
DESY, Hamburg
March 10, 2020

S2E with OCELOT

SRF-gun based: 100 pC, 7 GeV, ~5 kA, ~0.7 µm (partially optimized)

100 pC, 4 GeV, ~1.4 kA, ~0.5 µm

✓ **International efforts in CW regime:**

60th ICFA Advanced Beam Dynamics Workshop on Future Light Sources FLS2018, Shanghai, China JACoW Publishing
ISBN: 978-3-95450-206-6 doi:10.18429/JACoW-FLS2018-MOP1WA02

THE LCLS-II-HE, A HIGH ENERGY UPGRADE OF THE LCLS-II*

T.O. Raubenheimer†, for LCLS-II/LCLS-II-HE Collaborations
SLAC National Accelerator Laboratory, Menlo Park, USA

Abstract

The LCLS-II is a CW X-ray FEL covering a photon spectral range from 200 to 5,000 eV. It is based on a 4 GeV SRF linac installed in the 1st km of the SLAC linac tunnel. This paper will describe a high energy upgrade, referred to as the LCLS-II-HE, which will increase the beam energy to 8 GeV and the photon spectral range to 12.8 keV; this range may be extended through 20 keV with improvements of the electron injector and beam transport. The LCLS-II-HE received the US DOE CD-0 approval, Mission Need, and has developed a CDR in support of a CD-1 review scheduled for summer 2018.

portunities identified in the latest report from the Basic Energy Sciences Advisory Committee (BESAC) [4], and will provide detailed insight into the behavior of complex matter, real-world heterogeneous samples, functioning assemblies, and biological systems on fundamental scales of energy, time, and length. The LCLS-II High Energy Upgrade (LCLS-II-HE) is a natural extension to LCLS-II, extending the high-repetition-rate capabilities into the critically important "hard X-ray" regime (spanning from 5 keV to at least 12.8 keV and potentially up to 20 keV) that has been used in more than 75% of the LCLS experiments to date.

LCLS-II Beam and FEL Performance Based on Start-to-End Simulations Using a Gaussian-profile injector Laser

LCLS-II-TN-20-03

6/5/20 **S2E with various tools**

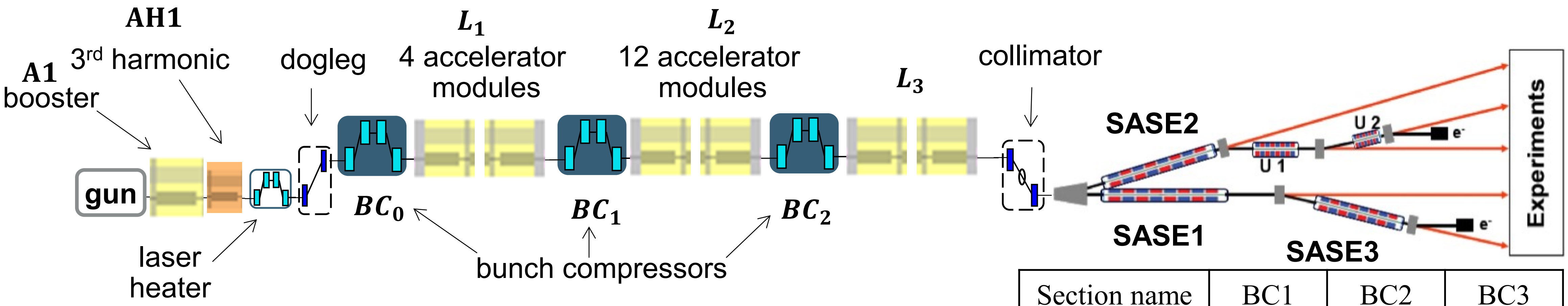
N. Neveu, N. Sudar, Y. Ding*, G. Marcus, A. Marinelli, C. Mayes
SLAC, Menlo Park, CA 94025, USA
J. Qiang **S2E with IMPACT**
LBNL, Berkeley, CA 94720, USA

Motivation & Goals

- **Optimizing injector**
- **Capability studies** of conserving e-bunch qualities through whole beamline
- **Finer S2E investigations** including micro bunching
- **Lasing performance** with optimized e-bunches before undulators

XFEL machine configuration

W. Decking et al, A MHz-repetition-rate hard X-ray free-electron laser driven by a superconducting linear accelerator, Nat. Photonics14, 391 (2020)



Section name	BC1	BC2	BC3
|r56|, mm	30-90	20-80	10-60

CW machine configuration staying same for current simulation studies

- **a high harmonic module** linearizing the longitudinal phase space
- **three bunch compressors** compressing the bunch to several kAs
- **design optics** providing a special phase advance between bunch compressors to reduce CSR

Energy gain budget in CW regime

- **First evaluation (E. Vogel):**
  - **16 MV/cavity** for 1.3 GHz
  - **4 MV/cavity** for 3.9 GHz
  - Beam energy at CW injector linac exit: **90 to 110 MeV**
  - Beam energy at BC1: **500 MeV**
  - Beam energy at BC2: **2 GeV**
  - Beam energy at exit of L3 (25 + 3 RF stations with 32 cavities each): **8 to 9 GeV**

- **A preliminary S2E energy profile for simulations**

  →110/500/2000/8000 MeV

- **A general optimization goal at a suitable S2E working point**

  →reasonably conserved central slice emittance;
  →kAs peak current & smooth profile;
  →reasonable slice energy spread before undulators.

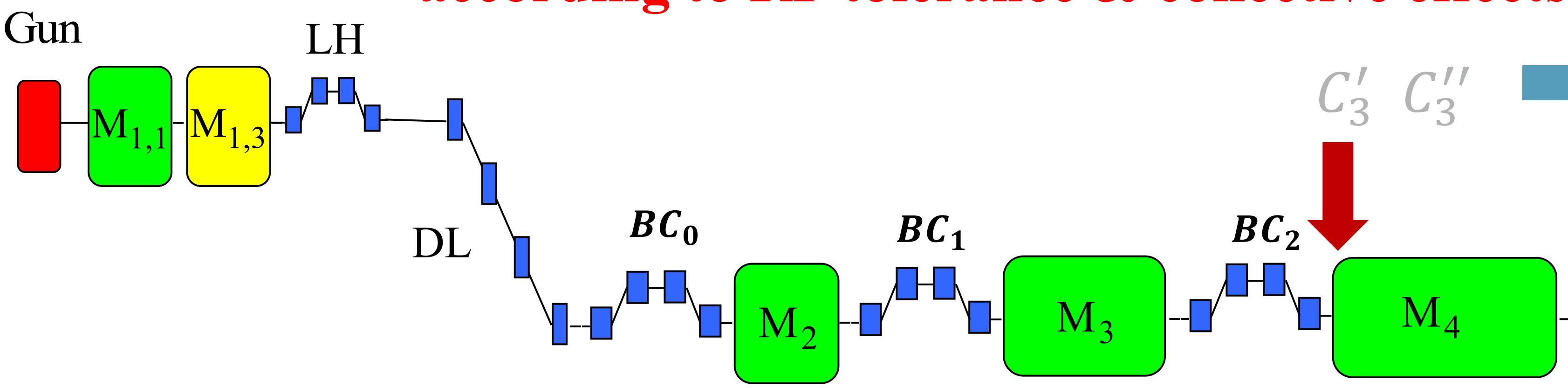
S2E BD with OCELOT

→ **searching working points for beam acceleration, transport & compression**

- → **stable compression**
- → **required bunch qualities before undulators**
- → **good SASE in hard X-ray regime**

Longitudinal beam dynamics optimization

Multi-parametric optimization according to RF tolerance & collective effects



the first and the second derivatives of the global compression

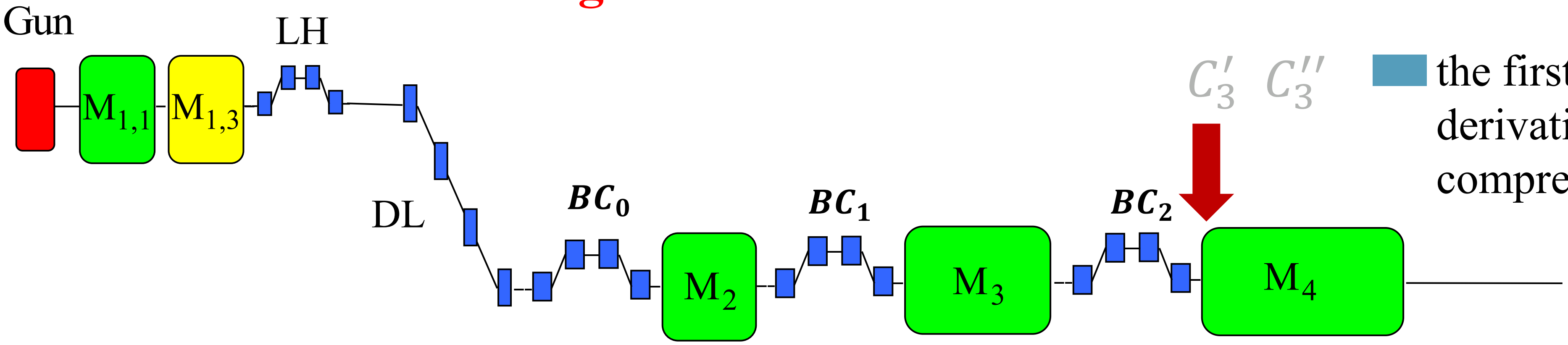
- energy in BC: E_1 = **110 MeV** E_2 = **500 MeV** E_3 = **2000 MeV**
- deflecting radius: $r_{56,1} = ?$ $r_{56,2} = ?$ $r_{56,3} = ?$
- compression factor: C_1 =? C_2 =? $C_3 = I_{\text{final}}/I_{\text{gun}}$

→ Searching for an optimal choice of parameters under technical constraints

e.g. E1/E2/E3→C3→C3′→r1→C1/C2/r2/r3→C3″

Longitudinal beam dynamics optimization

Multi-parametric optimization according to RF tolerance & collective effects



- the first and the second derivatives of the global compression

- energy in BC: E_1 = **110 MeV** E_2 = **500 MeV** E_3 = **2000 MeV**
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- compression factor: $C_1 = ?$ $C_2 = ?$ $C_3 = I_{\text{final}}/I_{\text{gun}}$

→ Searching for an optimal choice of parameters under technical constraints

→ Final bunch length & peak current sensitive to energy chirp, thus to RF parameters

Longitudinal beam dynamics optimization (cont'd)

PHYSICAL REVIEW ACCELERATORS AND BEAMS **22**, 024401 (2019)

Accelerator beam dynamics at the European X-ray Free Electron Laser

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The European X-Ray Free-Electron Laser Facility GmbH, 22869 Schenefeld, Germany

(Received 10 October 2018; published 13 February 2019)

$A(\boldsymbol{x}) = \boldsymbol{f},$

$\boldsymbol{f} = (E_1^0, E_2^0, E_3^0, Z_1, Z_2, Z_3, Z_3', Z_3''),$ → **BD** parameters

$\boldsymbol{x} = (X_{11}, Y_{11}, X_{13}, Y_{13}, X_2, Y_2, X_3, Y_3)$ → **RF** parameters

$\boldsymbol{x}_0 = A_0^{-1}(\boldsymbol{f})$ → analytical

tracking

$\boldsymbol{x}_n = A_0^{-1}(\boldsymbol{g}_n), \quad \boldsymbol{g}_n = \boldsymbol{g}_{n-1} + \lambda[\boldsymbol{f} - A(\boldsymbol{x}_{n-1})], \quad n > 0,$

$\boldsymbol{g}_0 = \boldsymbol{f}, \quad \boldsymbol{x}_0 = A_0^{-1}(\boldsymbol{f}).$ → iterative algorithm

→ **Searching suitable RF parameters *x* to produce desired compression scheme *f***

- → **Mapping RF parameters into longitudinal BD parameters**
- → **Realized by OCELOT**

A simulation toolkit: OCELOT

Courtesy: Sergey Tomin

ocelot-collab / ocelot

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master | 4 branches | 29 tags | Go to file | Add file | Code

sergey-tomin PEP warnings fixed — 8ce404a 3 days ago — 2,147 commits

demos	fixed some PEP warnings in PFS module	3 days ago
docs	Make sphinx documentation buildable	19 days ago
ocelot	PEP warnings fixed	3 days ago
ocelot_gui	update lat2input function in cpbd/io.py file	2 years ago
unit_tests	added bump utils and unit tests	4 days ago
.gitignore	Make sphinx documentation buildable	19 days ago
AUTHORS	corrected email	7 months ago
LICENSE	changed multiplication TM on Particle.	4 years ago
README.md	updated readme.md	4 days ago
setup.py	fixed some PEP warnings in PFS module	3 days ago

About

OCELOT is a multiphysics simulation toolkit designed for studying FEL and storage ring-based light sources.

accelerator-physics | fel | simulations | python | ocelot-collab | ocelot

S.Tomin, I.Agapov, M.Dohlus, I.Zagorodnov, *Ocelot as framework for beam dynamics simulations of x-ray sources, in Proceedings of IPAC 2017, WEPAB031*

A simulation toolkit: OCELOT

Courtesy: Sergey Tomin

An Introduction to Ocelot

Ocelot is a multiphysics simulation toolkit designed for studying FEL and storage ring-based light sources. Ocelot is written in Python. Its central concept is the writing of python's scripts for simulations with the usage of Ocelot's modules and functions and the standard Python libraries.

Ocelot includes following main modules:

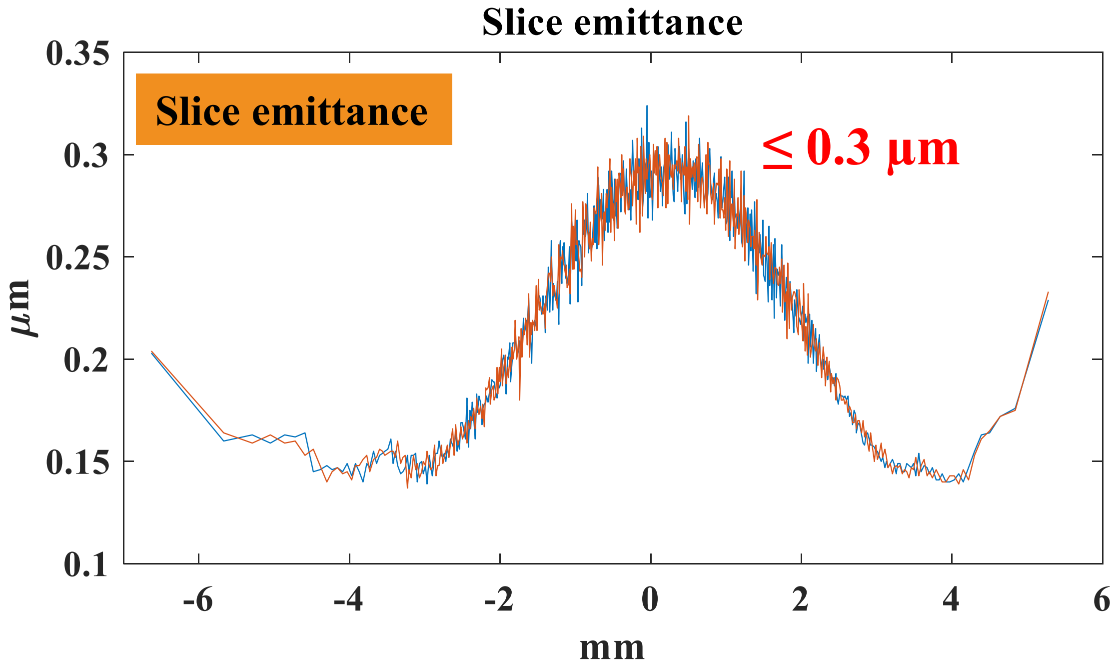
- **Charged particle beam dynamics module (CPBD)**
  - optics
  - tracking
  - matching
  - collective effects (description can be found here and here)
    - Space Charge (3D Laplace solver)
    - CSR (Coherent Synchrotron Radiation) (1D model with arbitrary number of dipoles).
    - Wakefields (Taylor expansion up to second order for arbitrary geometry).
  - MOGA (Multi Objective Genetics Algorithm) ref.
- **Native module for spontaneous radiation calculation** (some details can be found here and here)
- **FEL calculations: interface to GENESIS and pre/post-processing**
- **Modules for online beam control and online optimization of accelerator performances.** ref1, ref2, ref3, ref4.
  - This module is being developed in collaboration with other accelerator groups. The module has been migrated to a separate repository (in ocelot-collab organization) for ease of collaborative development.

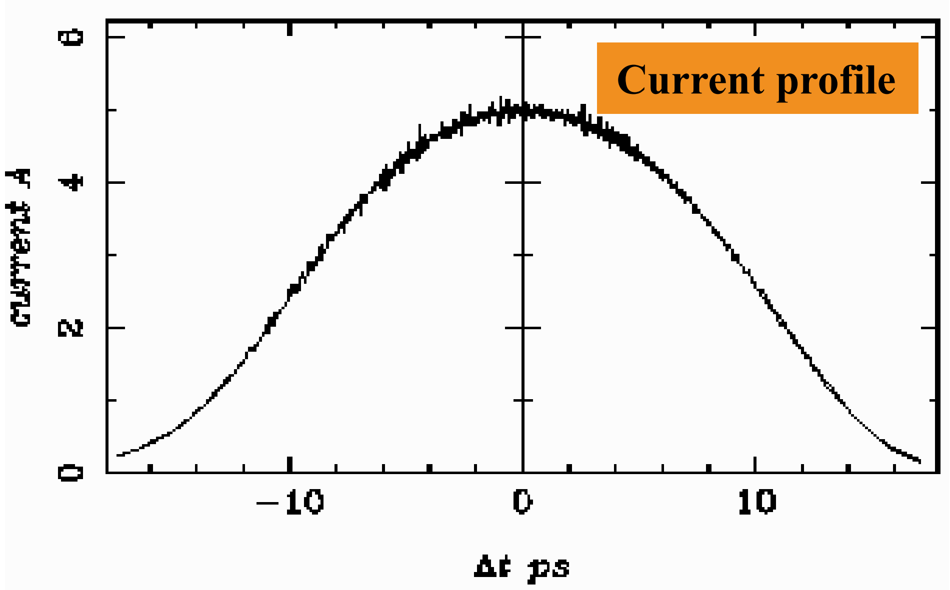
- **An iterative algorithm for searching RF parameters for compression studies also implemented in OCELOT**

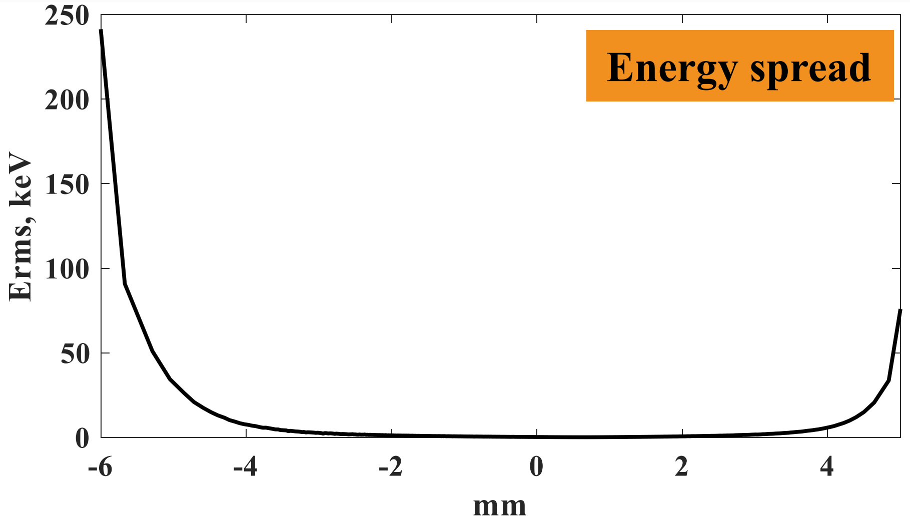
A fast estimation for S2E BD in OCELOT

→ injector bunches optimized by D. Bazyl

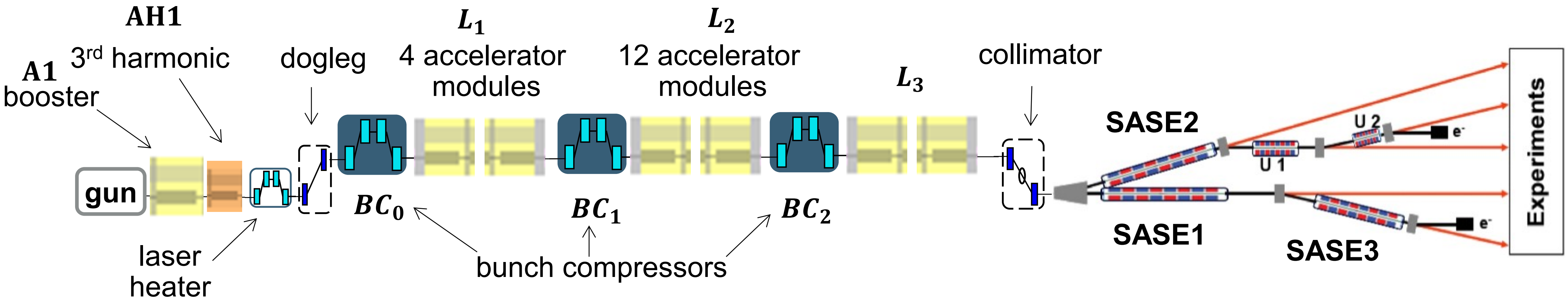
- Case study with one of the optimized bunches from the injector (emittance < 0.3 μm)







A fast estimation for S2E BD in OCELOT (cont'd)



- **A set of longitudinal beam dynamics parameters & a set of RF parameters aiming for ~3.5 kA at 100 pC, e.g.**

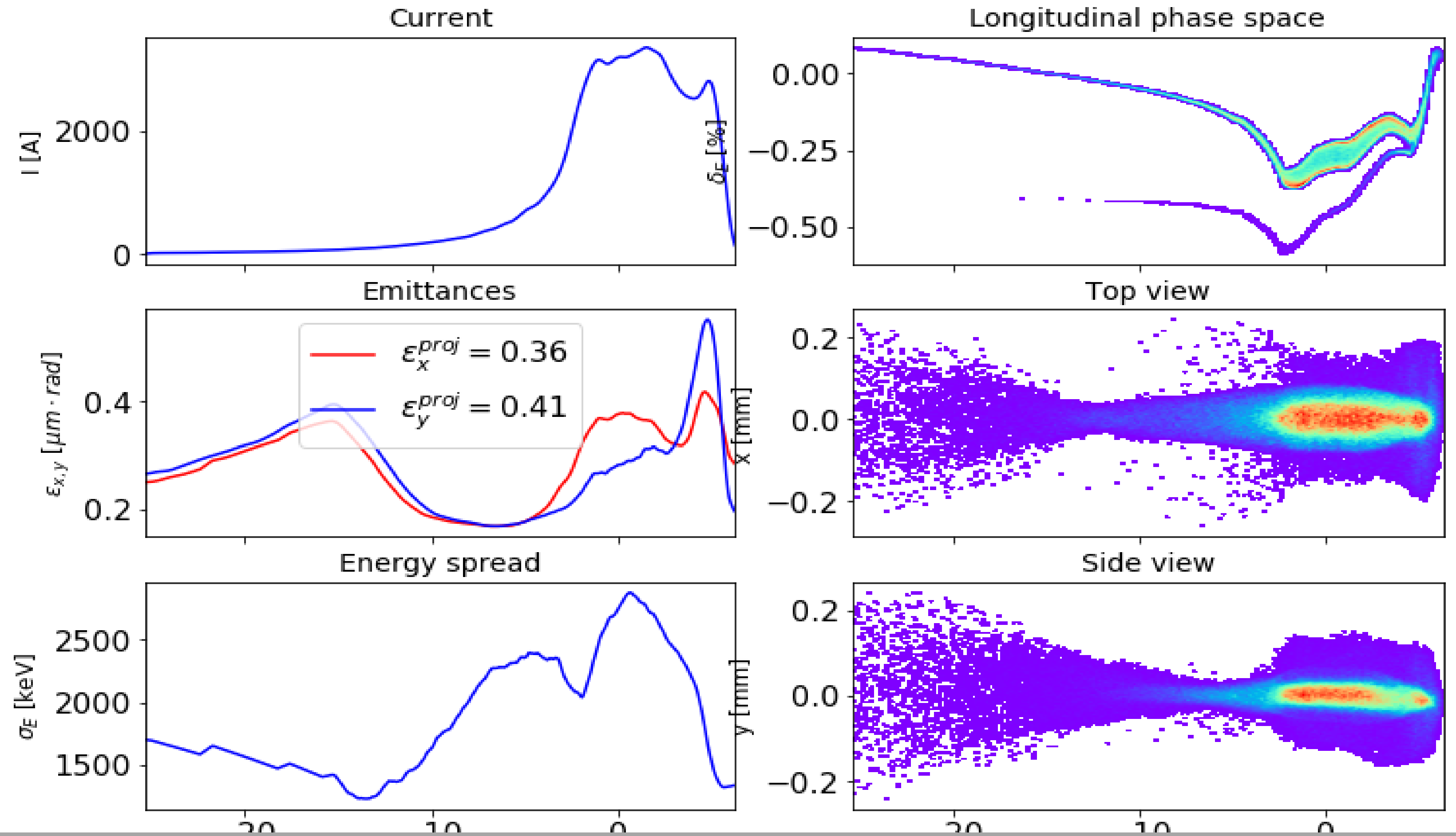
energy, MeV	110	500	2000
r56, mm	73.8	76.4	24.1
compression sp	3	30	700
with Z_3', 1/m = 0 & Z_3'', 1/m/m = 800			

The power of the LH model chosen to produce an energy modulation amplitude on axis & to have after compression an rms slice energy spread near to ~3 MeV based on dedicated μB studies

RF	V_{A1}, MV	φ_{A1}, deg	V_{AH1}, MV	φ_{AH1}, deg	V_{L1}, MV	φ_{L1}, deg	V_{L2}, MV	φ_{L2}, deg
	123.44	-7.462	20.01	153.41	414.89	19.93	1754	31.2

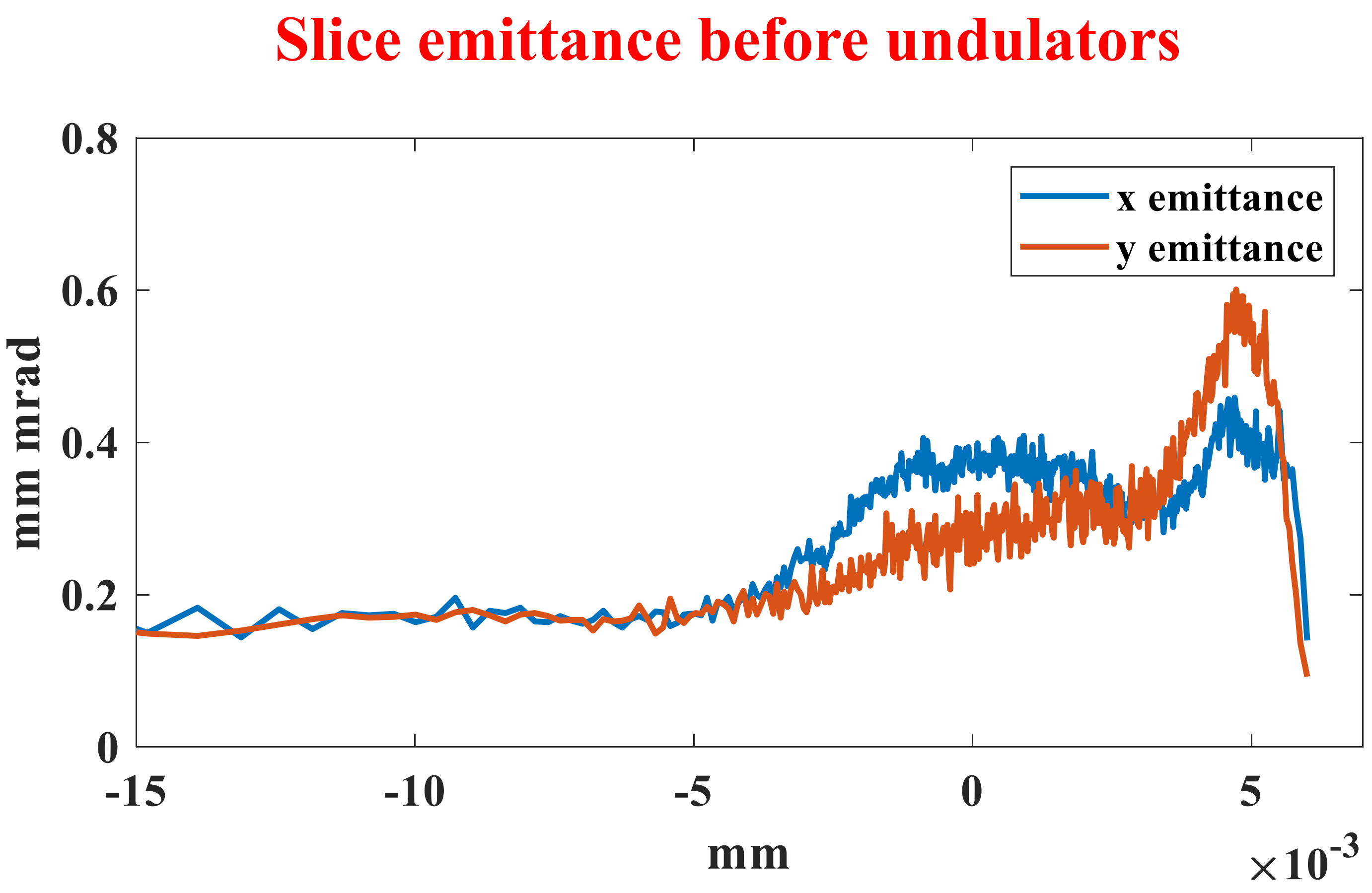
A fast estimation for S2E BD in OCELOT (cont'd)

→ particle distribution before SA1 (case of 3.5 kA)



NO micro bunching effect possibly considered in the simulations

A fast estimation for S2E BD in OCELOT (cont'd)



- First estimations by OCELOT showing for kAs' peak current the bunch quality before undulators can be ~conserved compared to that of the injector bunch without significant growth of central slice emittance

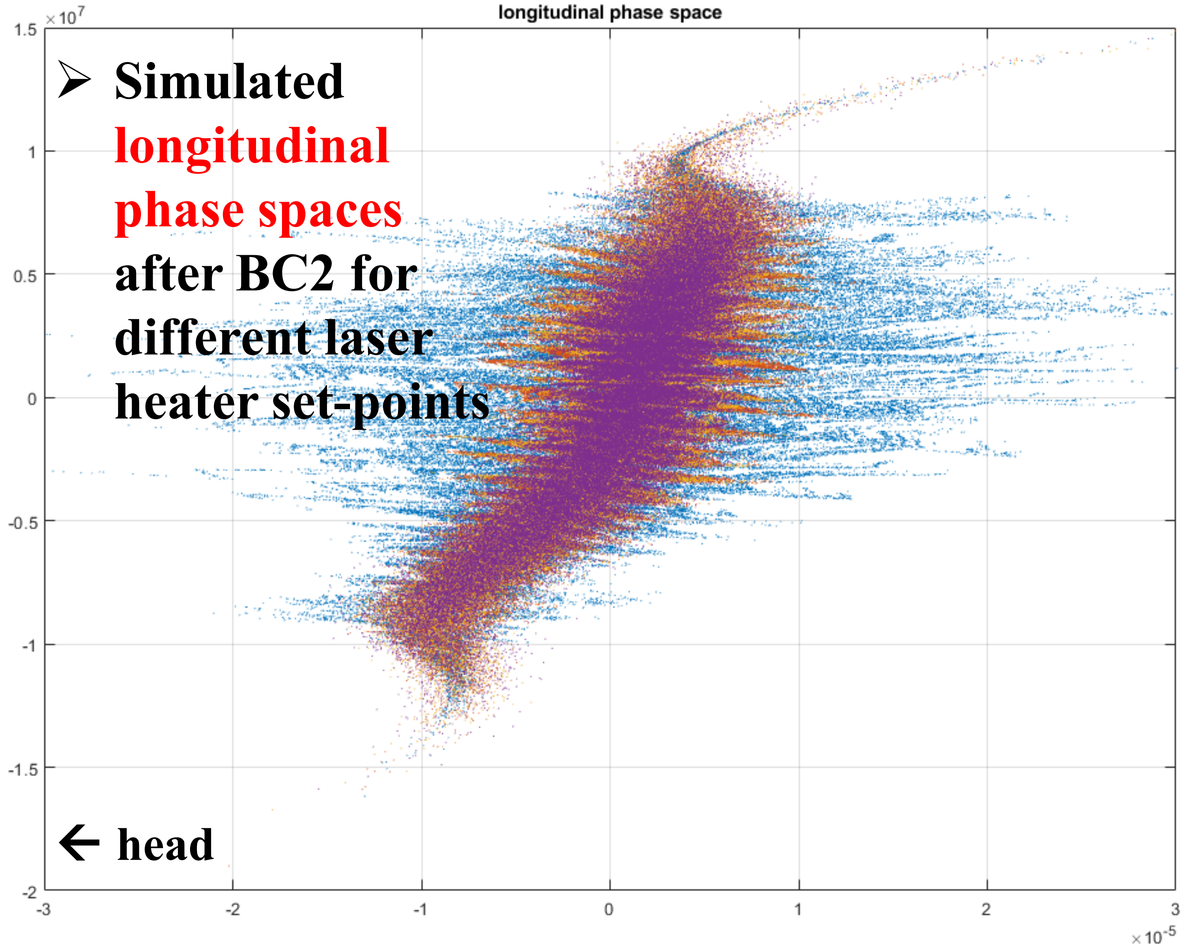
BD studies with Impact-Z (M. Dohlus)

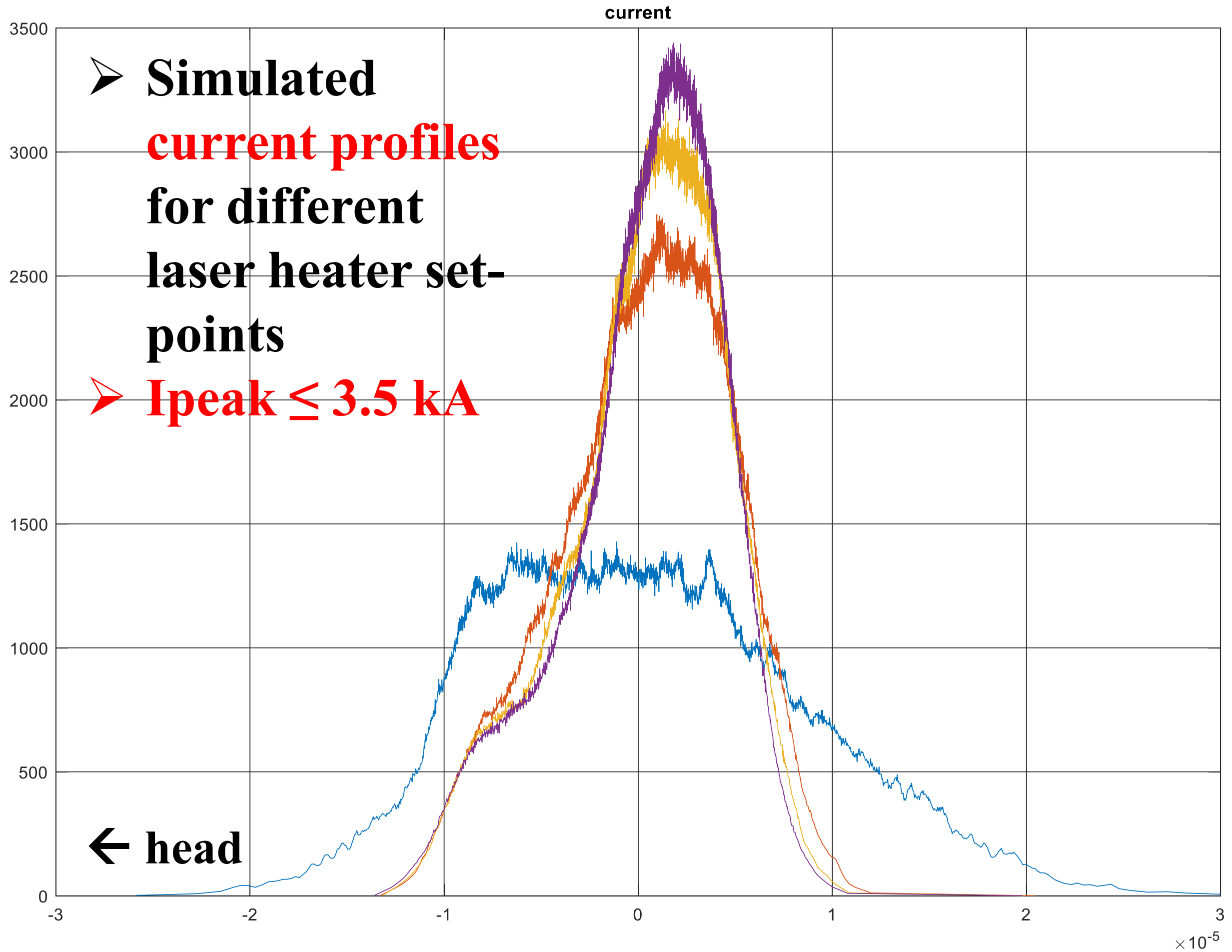
→ Microbunching effect

→ **ongoing** investigations with huge number of simulation particles & very fine numerical resolution

Fine Simulations with Impact-Z using 62 Millions macro particles for 100 pC (1 simulation particle ~ 10 electrons)

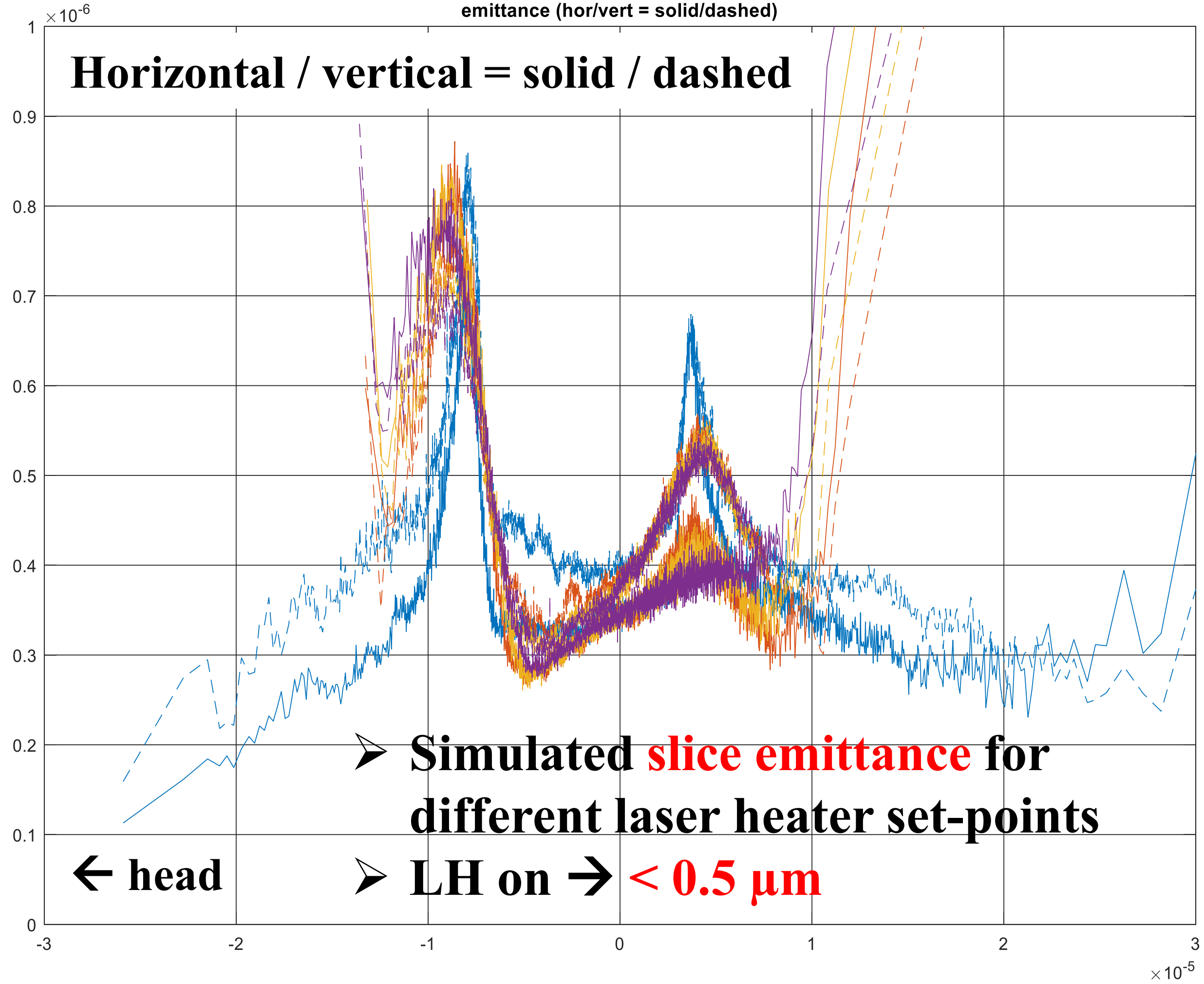
Laser Heater (LH) set-point: 0 eV/3300 eV/4000 eV/5000 eV

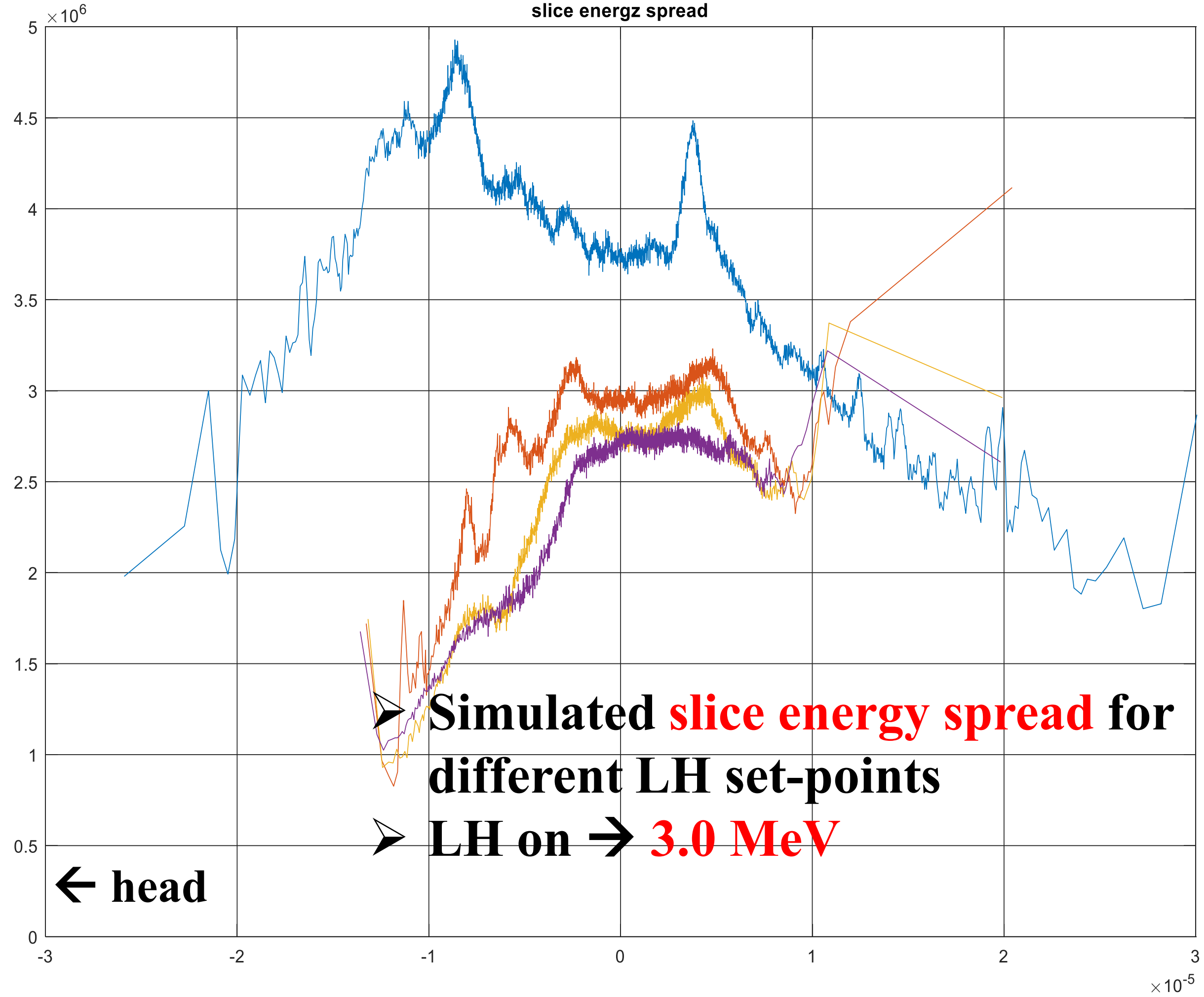




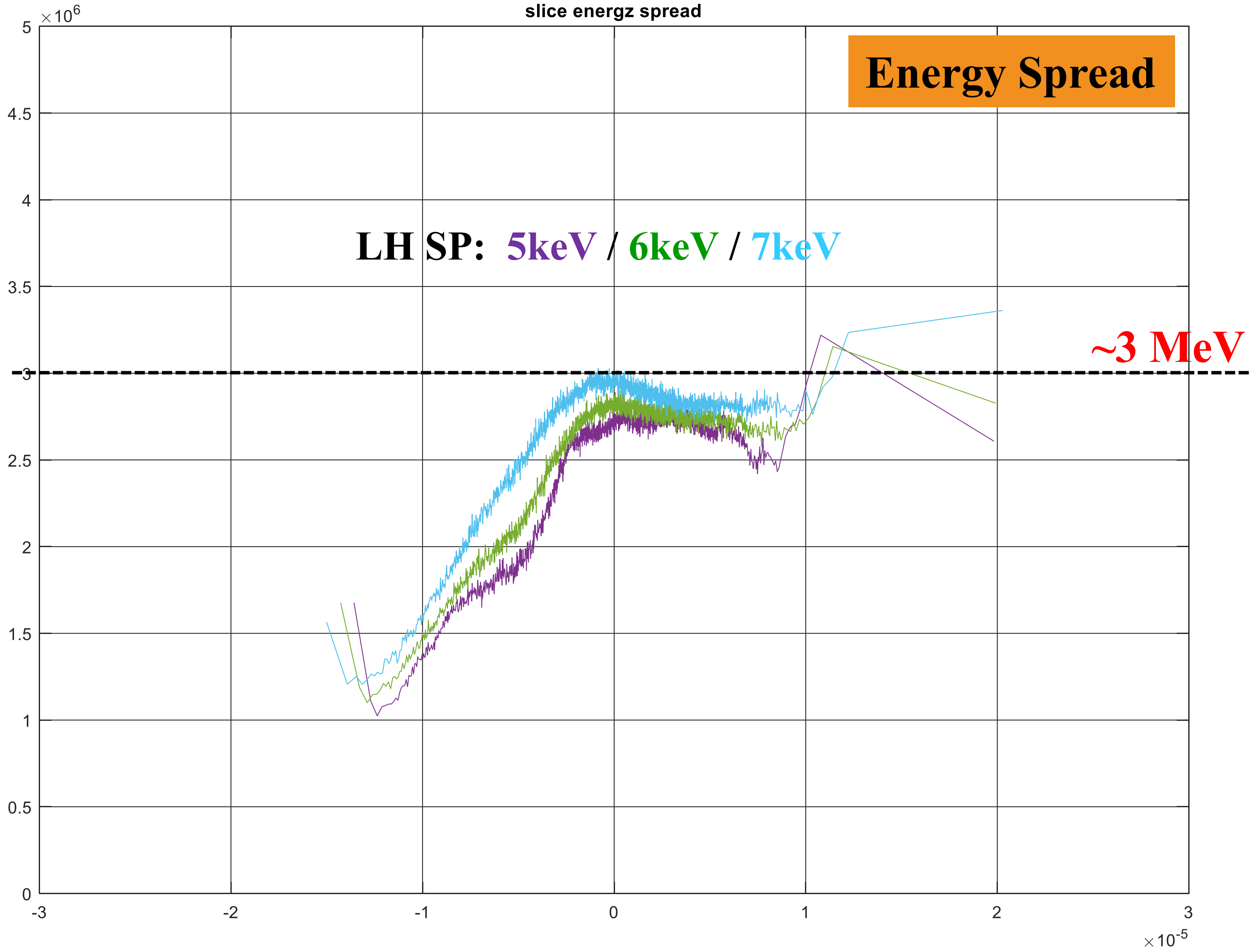
Fine Simulations with Impact-Z using 62 Millions macro particles (cont'd)

LH set-point: 0 eV/3300 eV/4000 eV/5000 eV

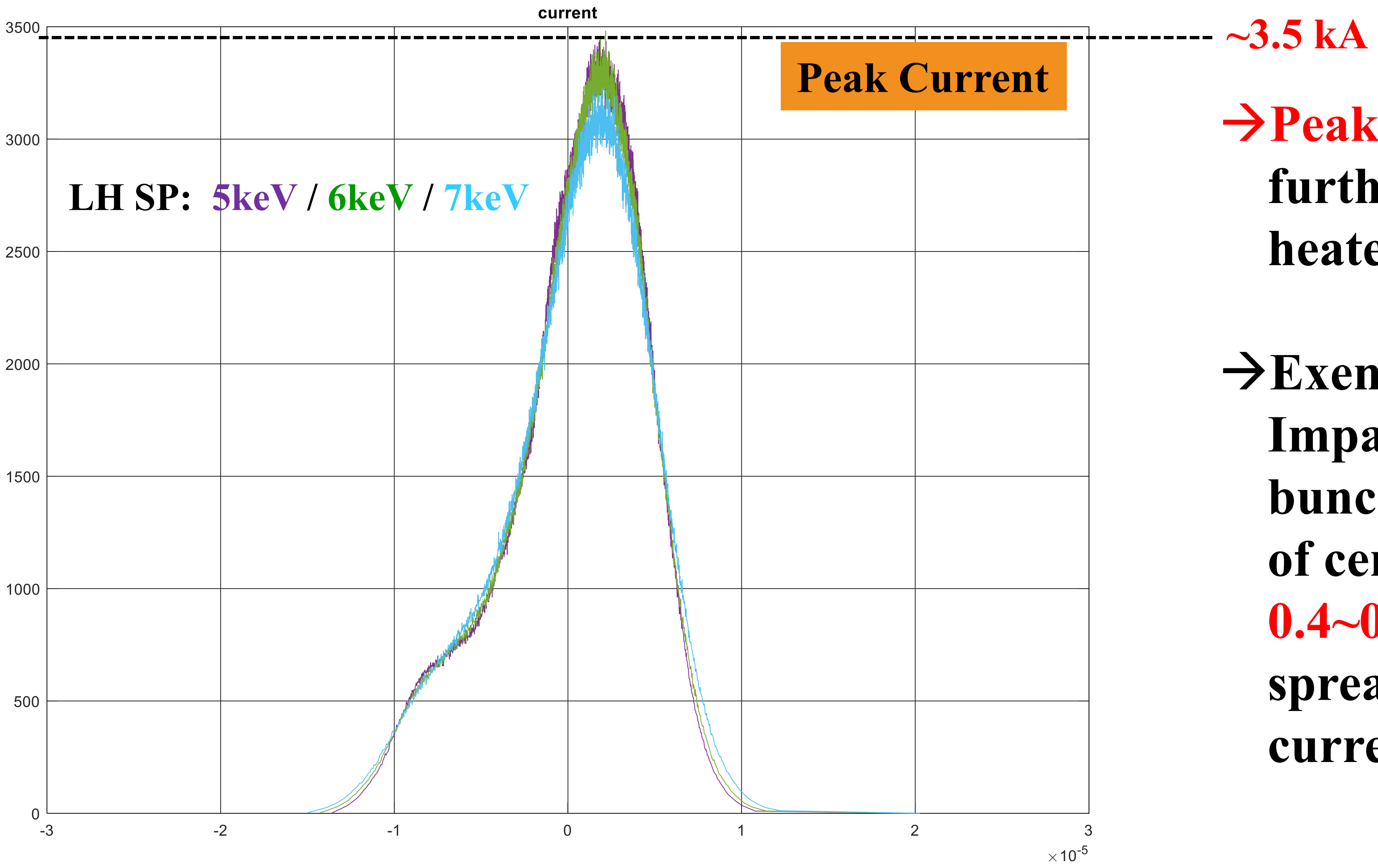




Fine Simulations with Impact-Z using 62 Millions macro particles (cont'd) → further increasing LH SP



Fine Simulations with Impact-Z using 62 Millions macro particles (cont'd) → further increasing LH SP

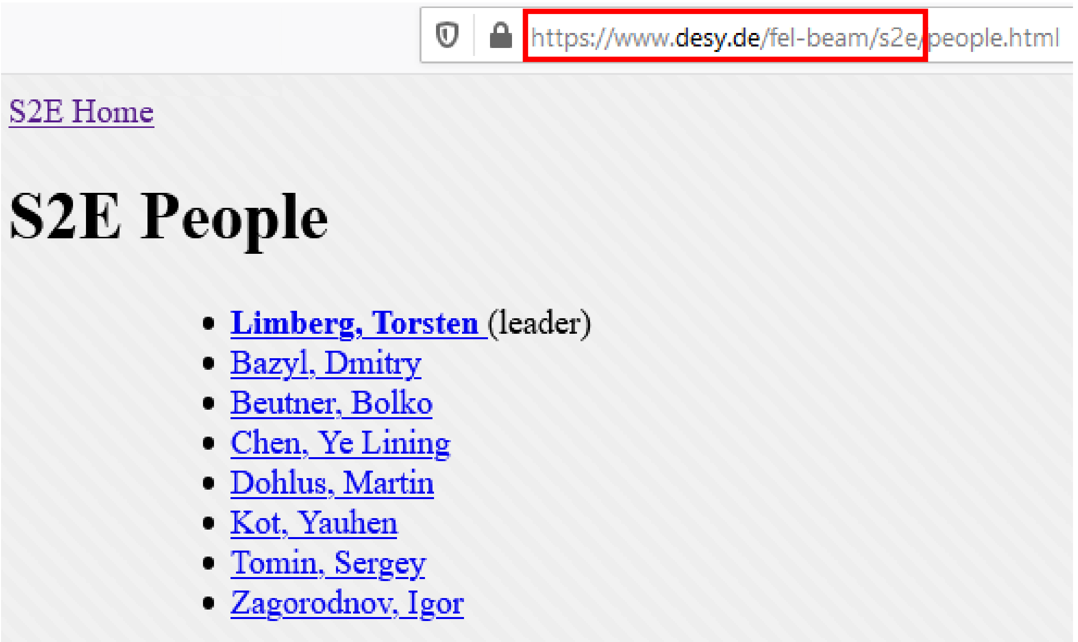


→**Peak current drops** as further increasing the laser heater set-point

→Exemplary case study in Impact-Z with micro bunching showing a bunch of central slice emittance **0.4~0.5 µm**, slice energy spread **~2.7 MeV** & peak current of **~ 3.5 kA**

Summary & Outlook

- **We started**
- **S2E BD studies** with optimized bunches from a SRF CW injector
  - → First results indicating **bunch quality can be conserved** before the undulator beamline **without significant growth of the central slice emittance** while being **compressed to ~kAs**
    - → Estimated by **OCELOT** w/o micro bunching
    - → Being simulated **by Impact-Z** with micro bunching (ongoing)
    - → Being simulated by **Xtrack** (ongoing)
    - → Warm-up lasing studies indicating **SASE signals** of mJ & hundreds µJ @ 0.24 & 0.17 nm w/o optimization or undulator modification (→ backup slides)


https://www.desy.de/fel-beam/s2e/people.html

S2E Home

S2E People

- **Limberg, Torsten** (leader)
- Bazyl, Dmitry
- Beutner, Bolko
- Chen, Ye Lining
- Dohlus, Martin
- Kot, Yauhen
- Tomin, Sergey
- Zagorodnov, Igor

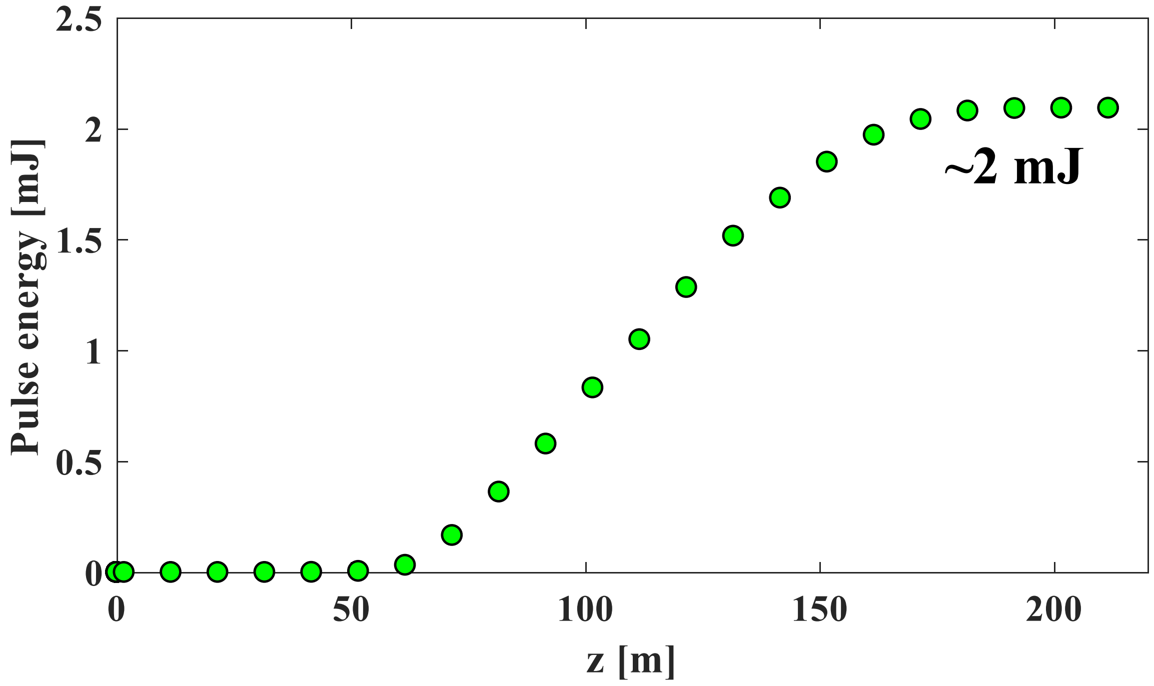
- **Work** towards CW regime
  - → **Injector** optimization
  - → **Compression** scenarios
  - → **Tool** studies for covering all collective effects properly
  - → Systematic **SASE** studies
  - → **Undulator** R&D, etc.

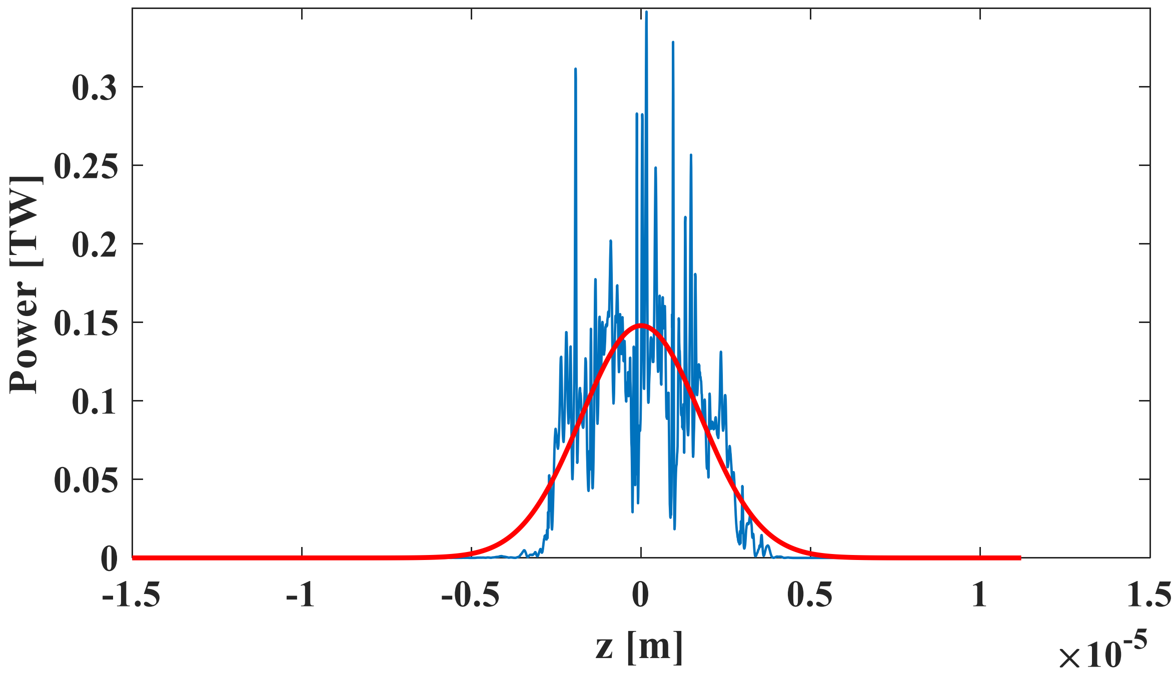
Backup Slides: SASE Simulations

Lasing @ 0.24 nm with the impact-Z bunch ("μB on") at a laser heater set-point of 5 keV

→ 100pC, ~8GeV, ~3.2kA, SA1

→ w/o any optimization or modification to undulator configuration

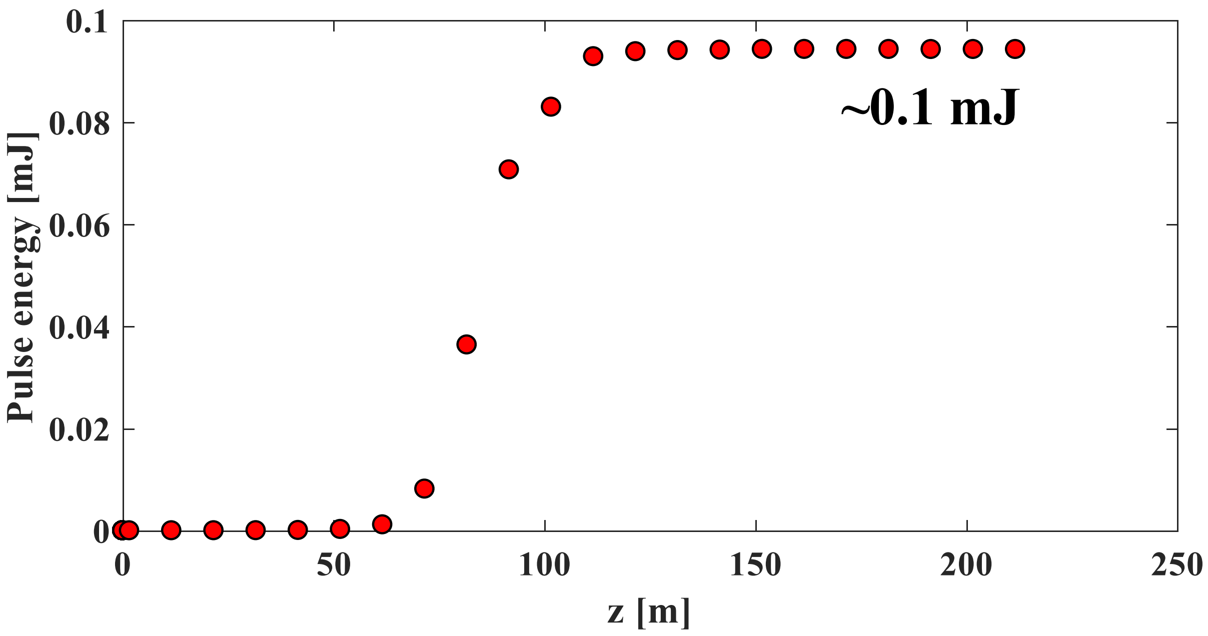


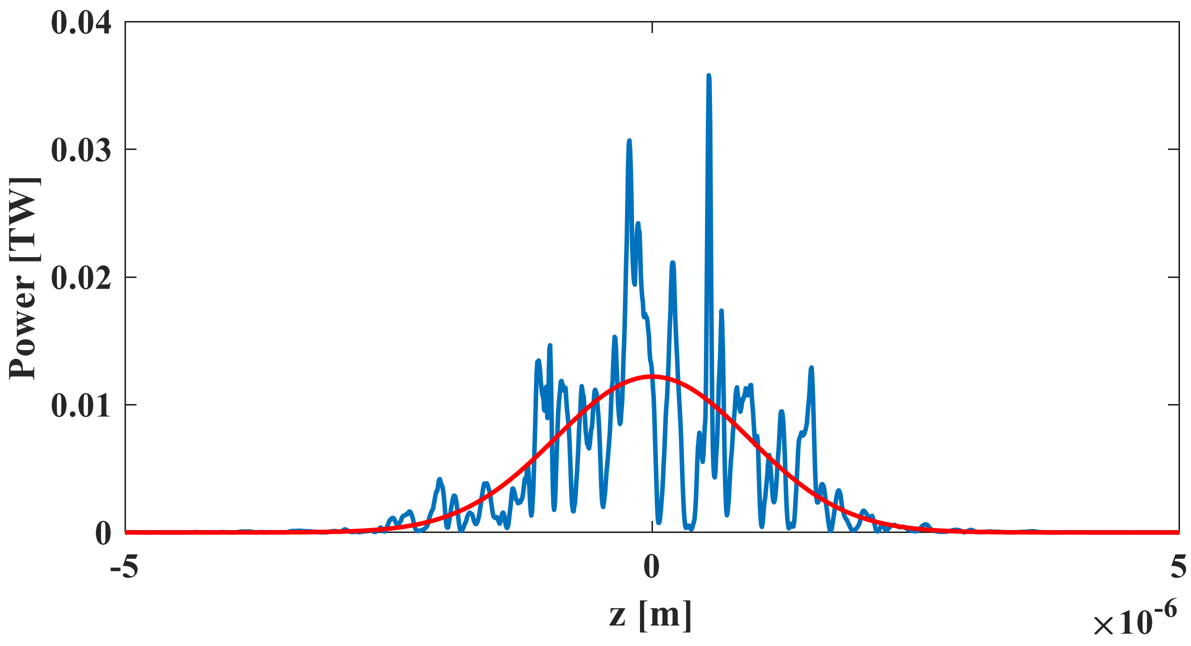


Lasing @ 0.17 nm with the impact-Z bunch ("μB on") at a laser heater set-point of 5 keV

→ 100pC, ~8GeV, ~3.2kA, SA1

→ w/o any optimization or modification to undulator configuration



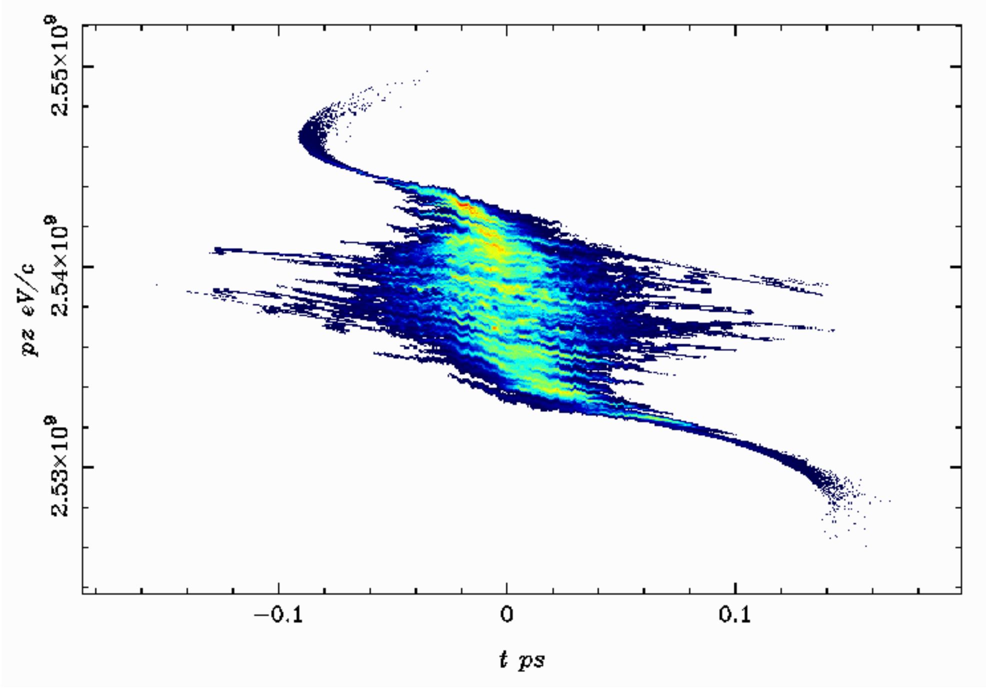


Laser heater impacts study for pulsed XFEL machine

→ 100pC, after BC2

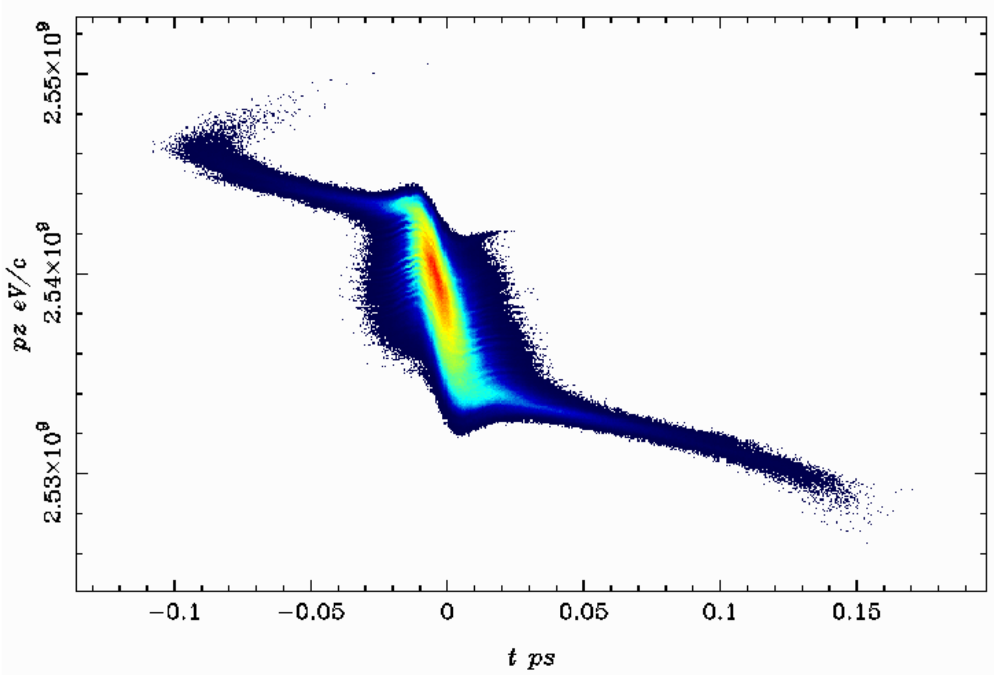
→ w/o any optimization or modification to undulator configuration

LPS w/o LH



- Peak current ~1.8 kA
- Central emittance ~ 0.5 µm
- Energy spread ~ 2 MeV

LPS w/ LH



- Peak current ~4.0 kA
- Central emittance ~ 0.5 µm
- Energy spread ~ 1.8 MeV

Laser heater impacts study for **pulsed** XFEL machine

→ 100pC, 14GeV, SA1

→ w/o any optimization or modification to undulator configuration

LH on, lasing@9keV

LH off → barely lases@9keV