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IBS Modeling in Reptil

Dec. 5, 2024, DESY



IBS in the XFEL injector

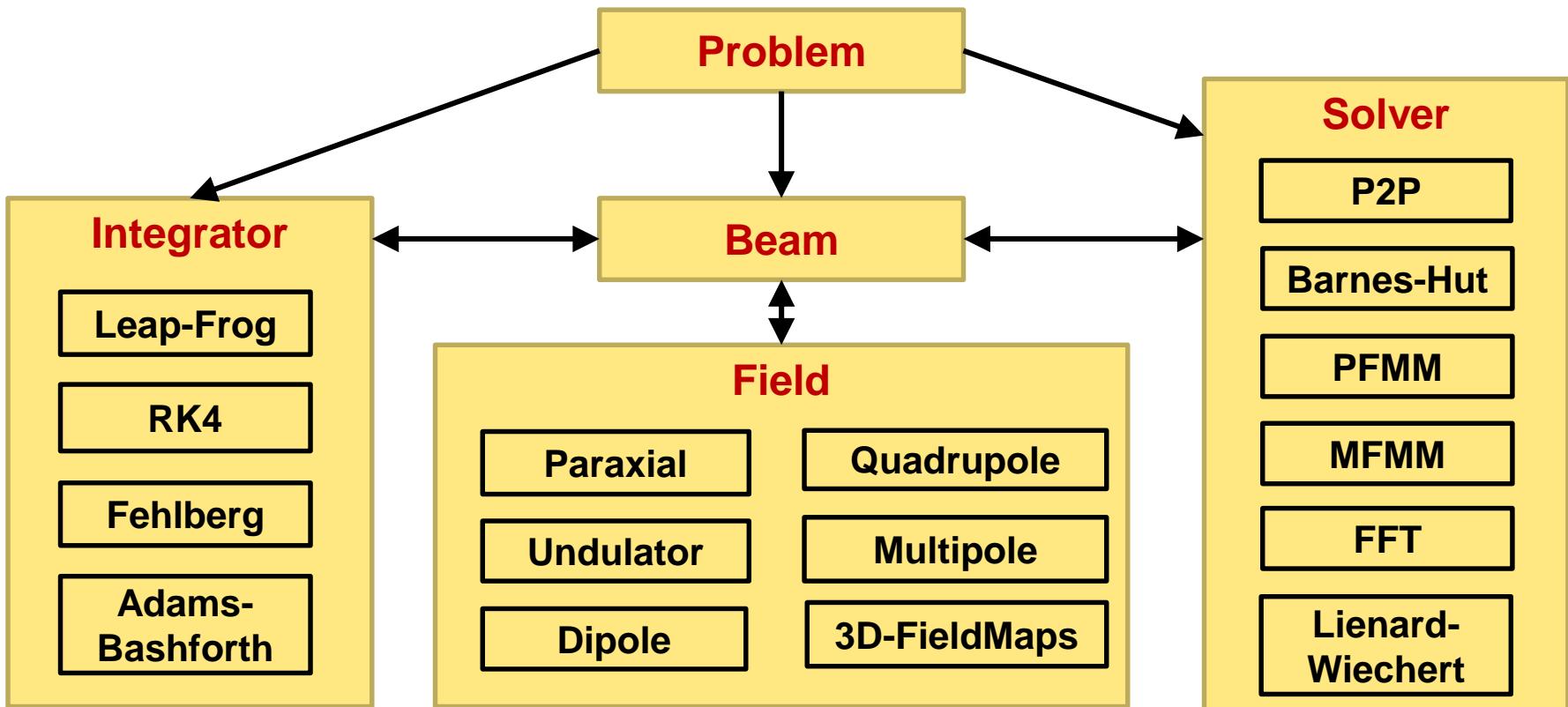


- The Reptil code
- IBS Model
- Validation studies
- Simulations
- Conclusions

The Reptil code



- RElativistic Particle Tracking for Injectors & Linacs

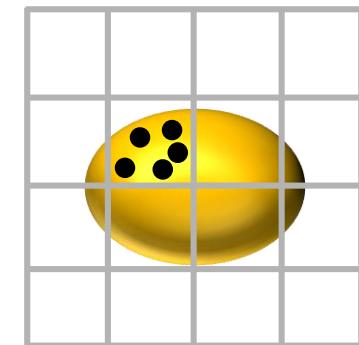
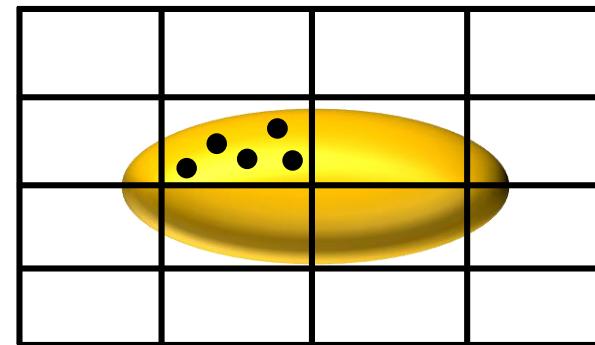
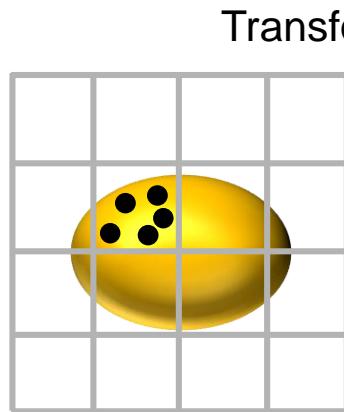


IBS Model in Reptil

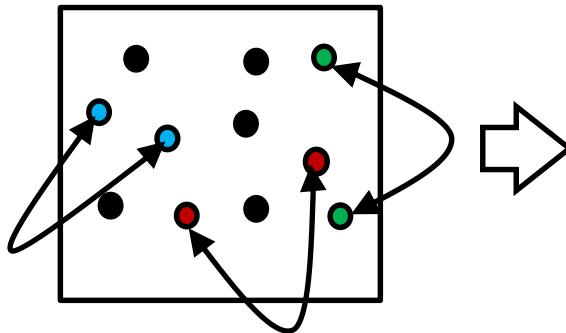


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DARMSTADT

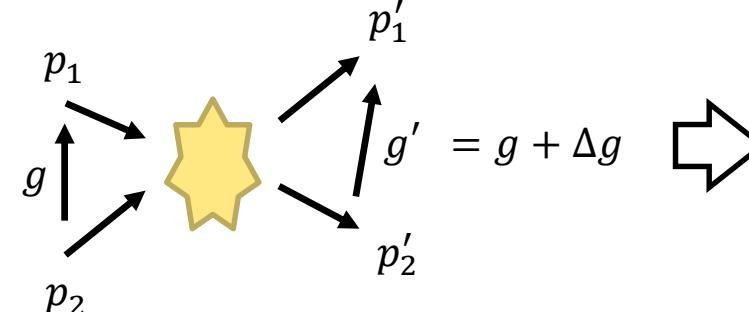
Monte-Carlo collisions (cell wise)



Build random particle pairs



Effective collision in the CM frame



Post-collision momenta

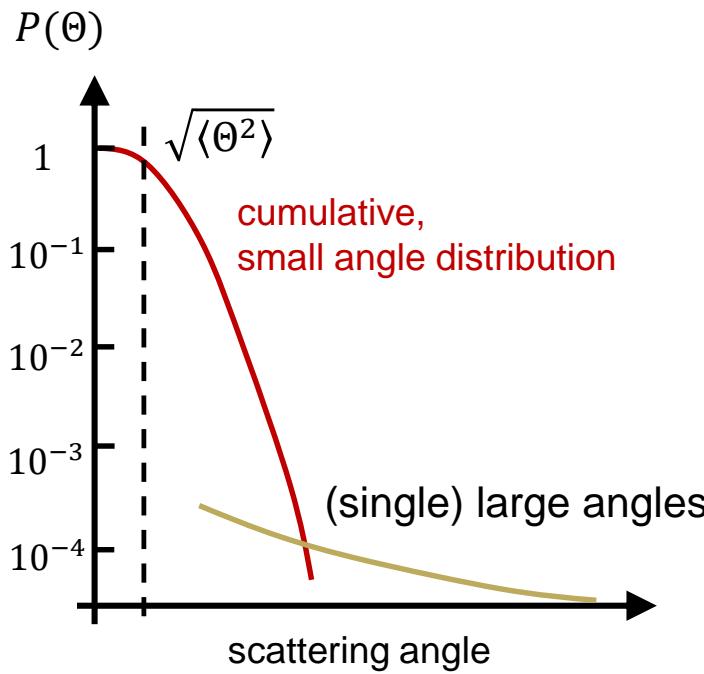
$$p_1' = p_1 + \frac{1}{2} \Delta g$$

$$p_2' = p_2 - \frac{1}{2} \Delta g$$

IBS Model in Reptil



▪ Cumulative scattering angle



For a single (binary) scattering angle event:

$$\langle \theta^2 \rangle = \frac{\int_{\theta_{min}}^{\theta_{max}} d\theta \sin(\theta) \theta^2 \frac{d\sigma(g, \theta)}{d\Omega}}{\int_{\theta_{min}}^{\theta_{max}} d\theta \sin(\theta) \frac{d\sigma(g, \theta)}{d\Omega}} = 2\theta_{min}^2 \ln\left(\frac{\theta_{max}}{\theta_{min}}\right)$$

$$\Lambda_c = \ln\left(\frac{\theta_{max}}{\theta_{min}}\right) \approx \ln\left(\frac{b_{max}}{b_{min}}\right)$$

Coulomb log.

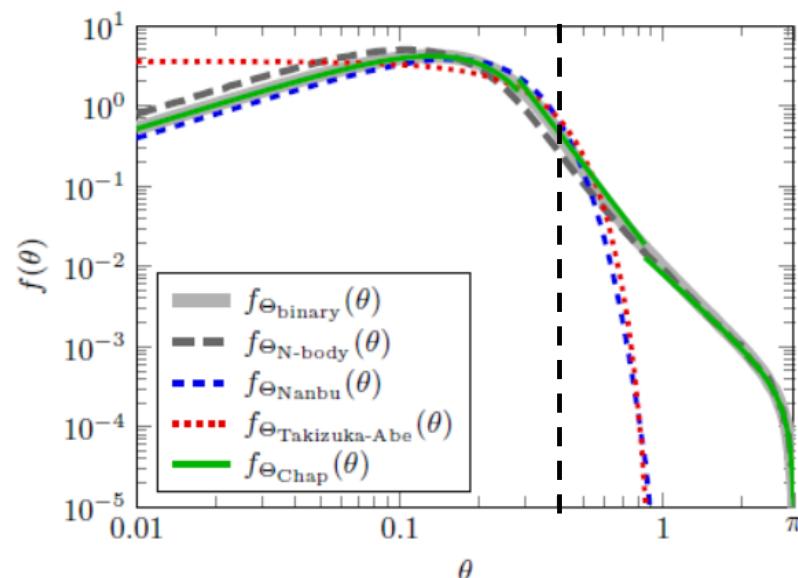
For N (large) scattering events → cumulative angle:

$$P(\Theta) \sim \frac{1}{\sqrt{(2\pi\langle\theta^2\rangle)}} e^{-\frac{\Theta^2}{2\langle\theta^2\rangle}}$$

$$\langle\theta^2\rangle = N\langle\theta^2\rangle \quad \text{with: } N = \pi b_{max}^2 n g \Delta t$$



- Cumulative scattering angle



Chap & Sedwick, Phys. Rev. E 95,
063209, 2017

For a single (binary) scattering angle event:

$$\langle \theta^2 \rangle = \frac{\int_{\theta_{min}}^{\theta_{max}} d\theta \sin(\theta) \theta^2 \frac{d\sigma(g, \theta)}{d\Omega}}{\int_{\theta_{min}}^{\theta_{max}} d\theta \sin(\theta) \frac{d\sigma(g, \theta)}{d\Omega}} = 2\theta_{min}^2 \ln\left(\frac{\theta_{max}}{\theta_{min}}\right)$$

$$\Lambda_c = \ln\left(\frac{\theta_{max}}{\theta_{min}}\right) \approx \ln\left(\frac{b_{max}}{b_{min}}\right)$$

Coulomb log.

Nanbu's correction for finite N:

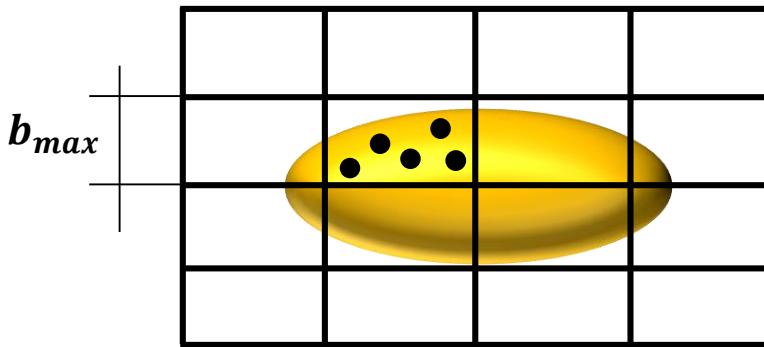
- Solve $\coth(A) - A^{-1} = \exp(-2\langle \theta^2 \rangle)$
- Generate cumulative angle as:

$$\theta(u) = \arccos \{ \log[\exp(-A) + 2 u \sinh(A)] \}$$
with $u \in [0,1]$

IBS Model in Reptil

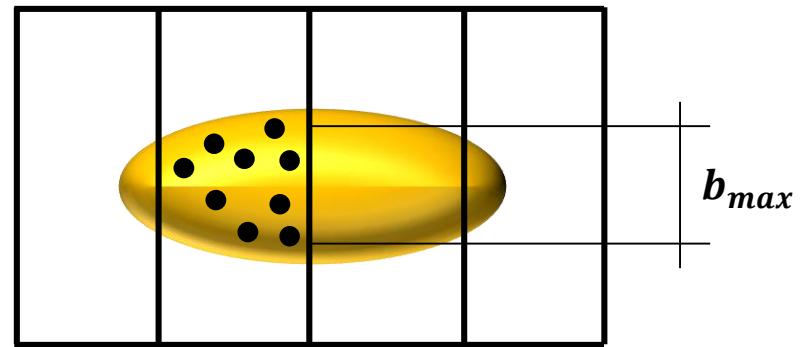
- Choice of Coulomb logarithm

Group particles by cell



Sensitive to mesh refinement!

Group particles by slice



Assumes uniform density in slice!

Shortcomings:

- Does not resolve transverse density variations
- Longitudinal collisions (at very low energies) not included
- Correction for the distribution tail at large angles might be needed → Coulomb log.
- This heuristics cannot be avoided in simulations as well as analytical models**

Validation studies

- The original Piwinski model:

$$\frac{1}{\tau_\delta} = \frac{1}{\sigma_\delta} \frac{d\sigma_\delta}{dt} = \frac{2r_e c N_b}{64\pi^2 \beta^3 \gamma^2 \epsilon_x^n \epsilon_y^n \sigma_z \sigma_\delta} f \left(\frac{\sigma_\delta}{\gamma \sigma_{x'}}, \frac{\sigma_\delta}{\gamma \sigma_{y'}}, 2\sigma_\delta \beta \sqrt{\frac{\sigma_y}{r_e}} \right)$$

- The high-energy approximation for round beams (Huang, Bane, 2002):

$$\frac{1}{\tau_\delta} = \frac{1}{\sigma_\delta} \frac{d\sigma_\delta}{dt} = \frac{r_e^2 c N_b \Lambda_c}{8 \epsilon_x^n \epsilon_x^n \sigma_x \sigma_z \gamma^2 \sigma_\delta^2},$$

$$\Lambda_c = \ln \left(\frac{\Delta \gamma_{max}}{\Delta \gamma_{min}} \right) = \ln \frac{\sigma_x}{\underbrace{r_e / (\gamma^2 \sigma_{x'}^2)}_{b_{min}}} \rightarrow \color{red} b_{max}$$

„Cutting“ the tail of scattering angle distribution (Huang, 2002):

$$\Delta \gamma_{max} \sim \gamma \times 10^{-5} \rightarrow \Lambda_c = \ln \left(\frac{\epsilon_x^n \times 10^{-5}}{r_e} \right) \approx 8 \quad \text{for } \epsilon_x^n = 1 \mu m$$

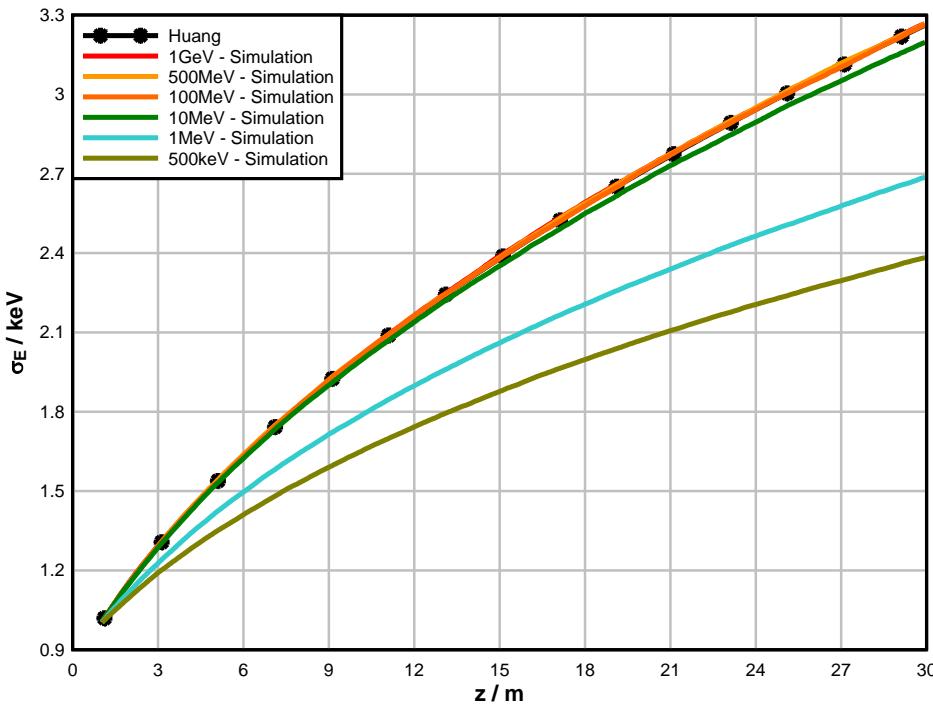
This value is wrongly used in several recent papers

Validation studies

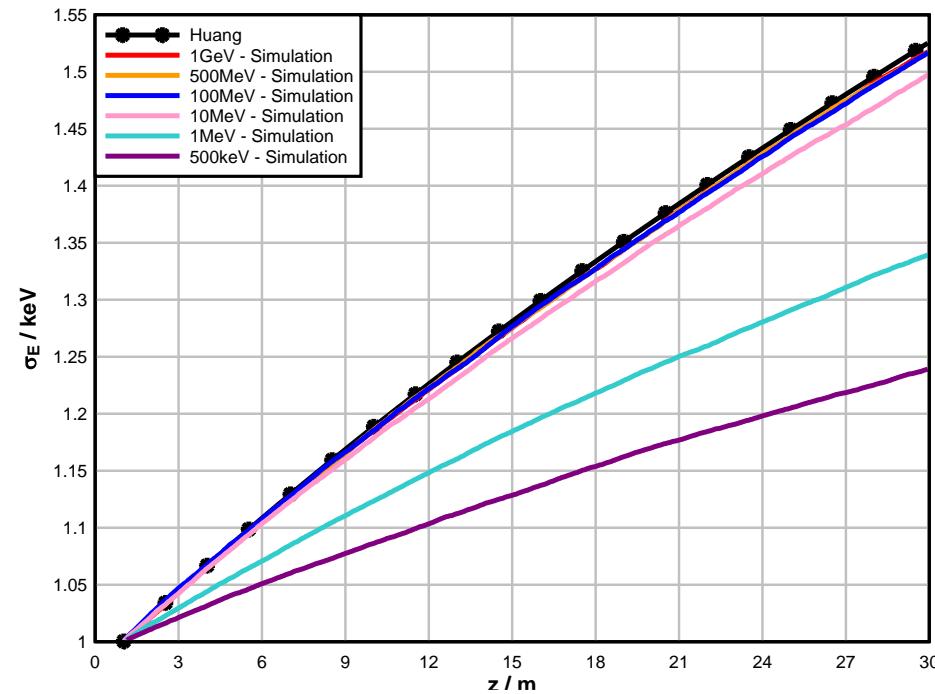


- IBS growth for frozen beam: $\epsilon_x^n = 1\mu m$, $\sigma_x = 250\mu m$, $\sigma_z = 1mm$

Pencil beam



Gaussian beam



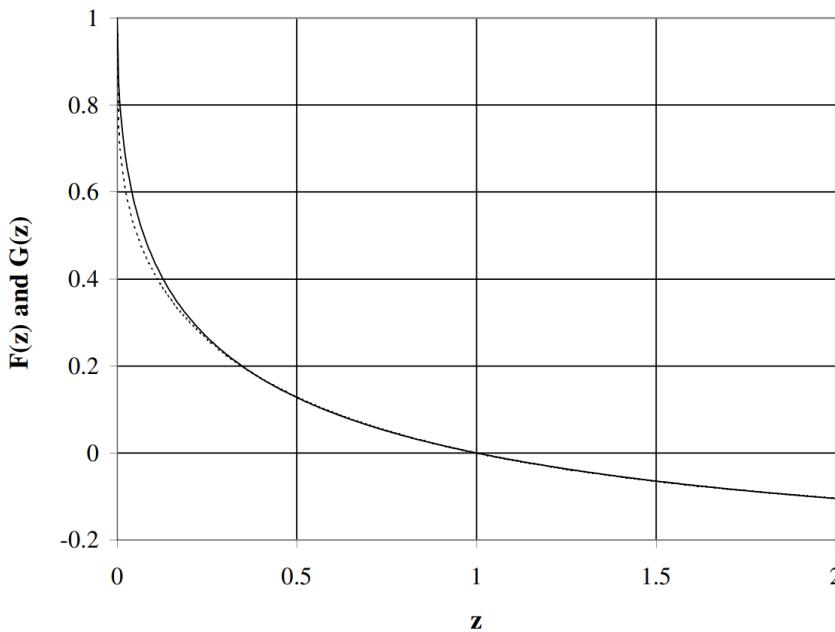
Validation studies



- Low energy IBS fitting formula (Nagaitev, 2005):

$$\frac{1}{\tau_\delta} = \frac{1}{\sigma_\delta} \frac{d\sigma_\delta}{dt} = \frac{r_e^2 c N_b \Lambda_c}{8\beta^3 \epsilon_x^n \epsilon_x^n \sigma_x \sigma_z \gamma^2 \sigma_\delta^2} \cdot F(\xi)$$

$$\xi = \left(\frac{\sigma_\delta \sigma_x}{\epsilon_x^n} \right)^2 = \left(\frac{\sigma_\gamma \sigma_x}{\gamma \epsilon_x^n} \right)^2$$



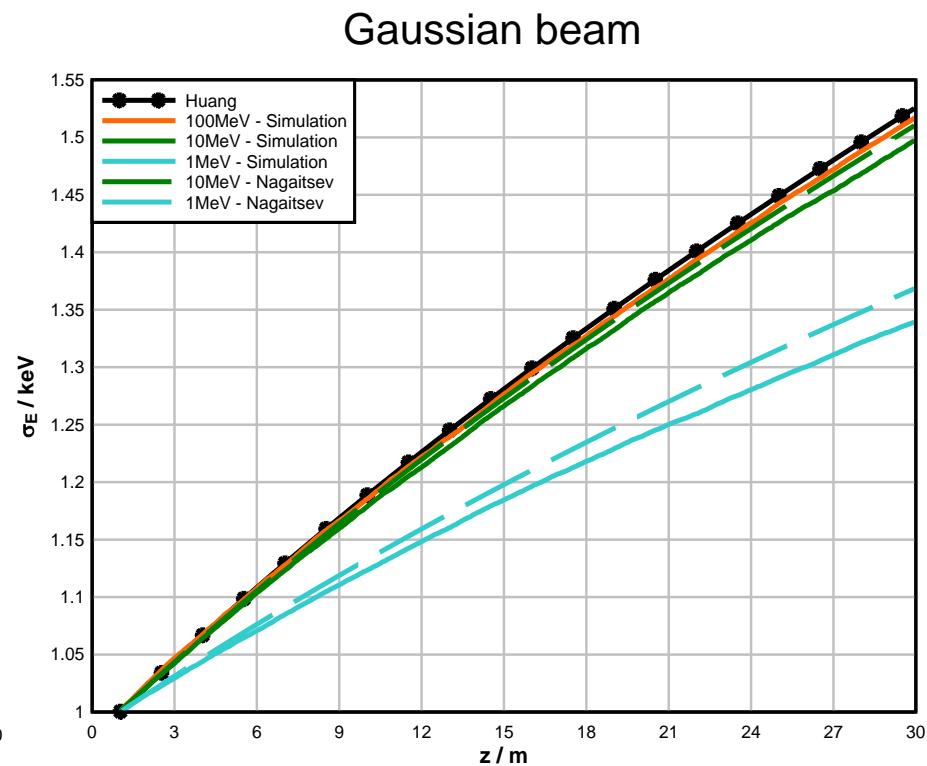
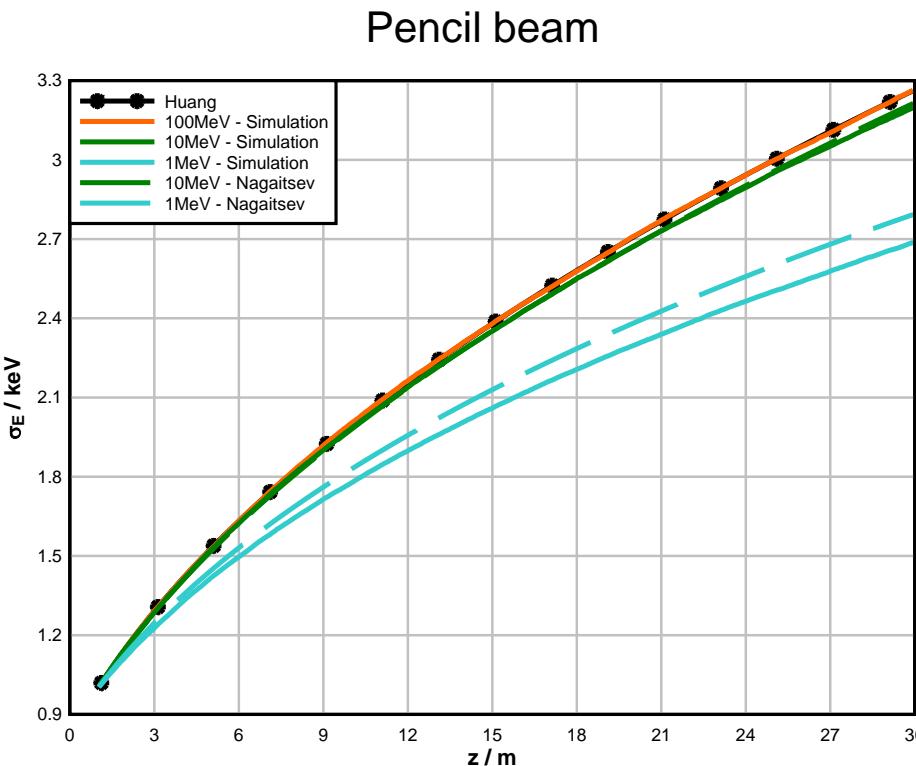
$$F(\xi) \approx G(\xi) = (1 - \xi^4) \frac{\ln(\xi + 1)}{\xi}$$

S. Nagaitev, PRST-AB, 8, 064403 (2005)

Validation studies

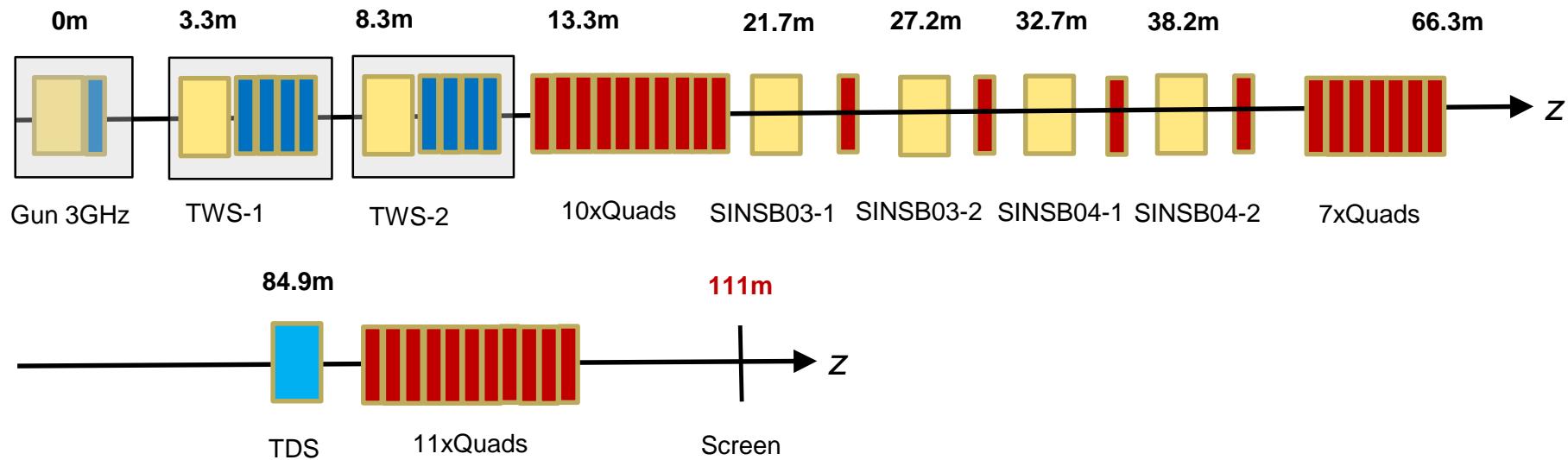


- IBS growth for frozen beam: $\epsilon_x^n = 1\mu m$, $\sigma_x = 250\mu m$, $\sigma_z = 1mm$





- The SwissFEL injector

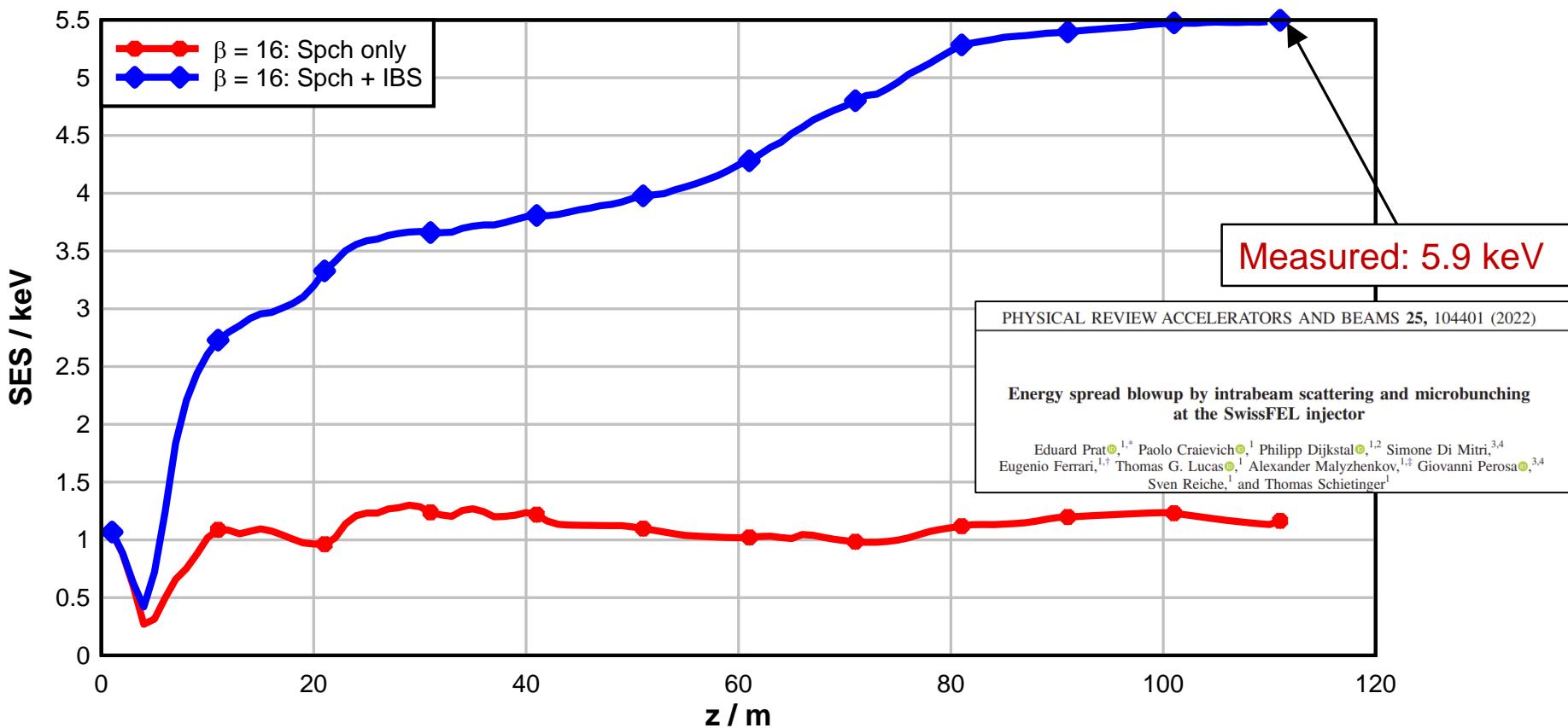


- Final energy: 320 MeV
- Bunch charge: 10...200 pC (nominal 200 pC)
- Average β -function: ~ 16 m (nominal)
- Bunch compressor and laser heater switched off ($R_{56}=0$)

Simulations for the SwissFEL

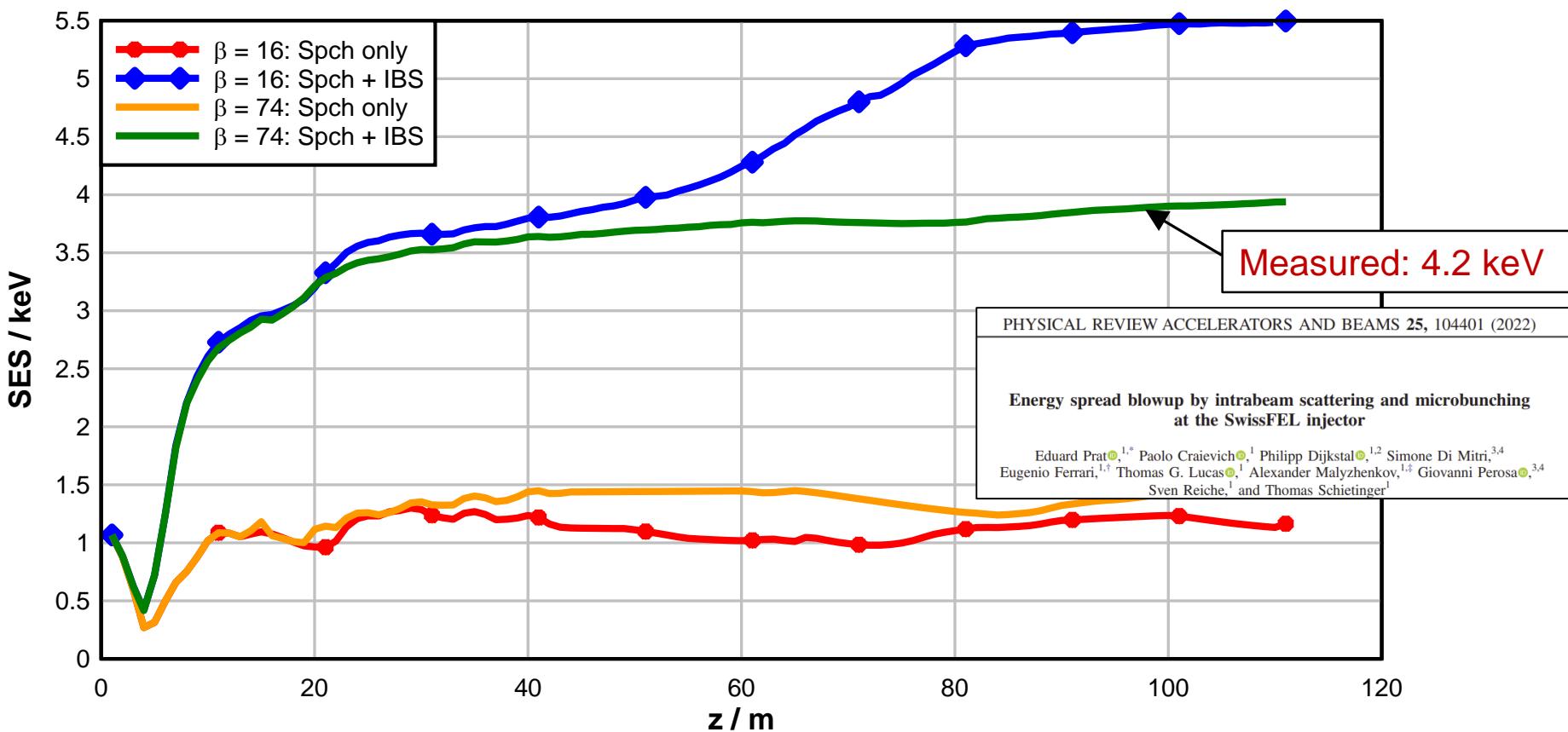


- Slice energy spread (nominal configuration)



Simulations for the SwissFEL

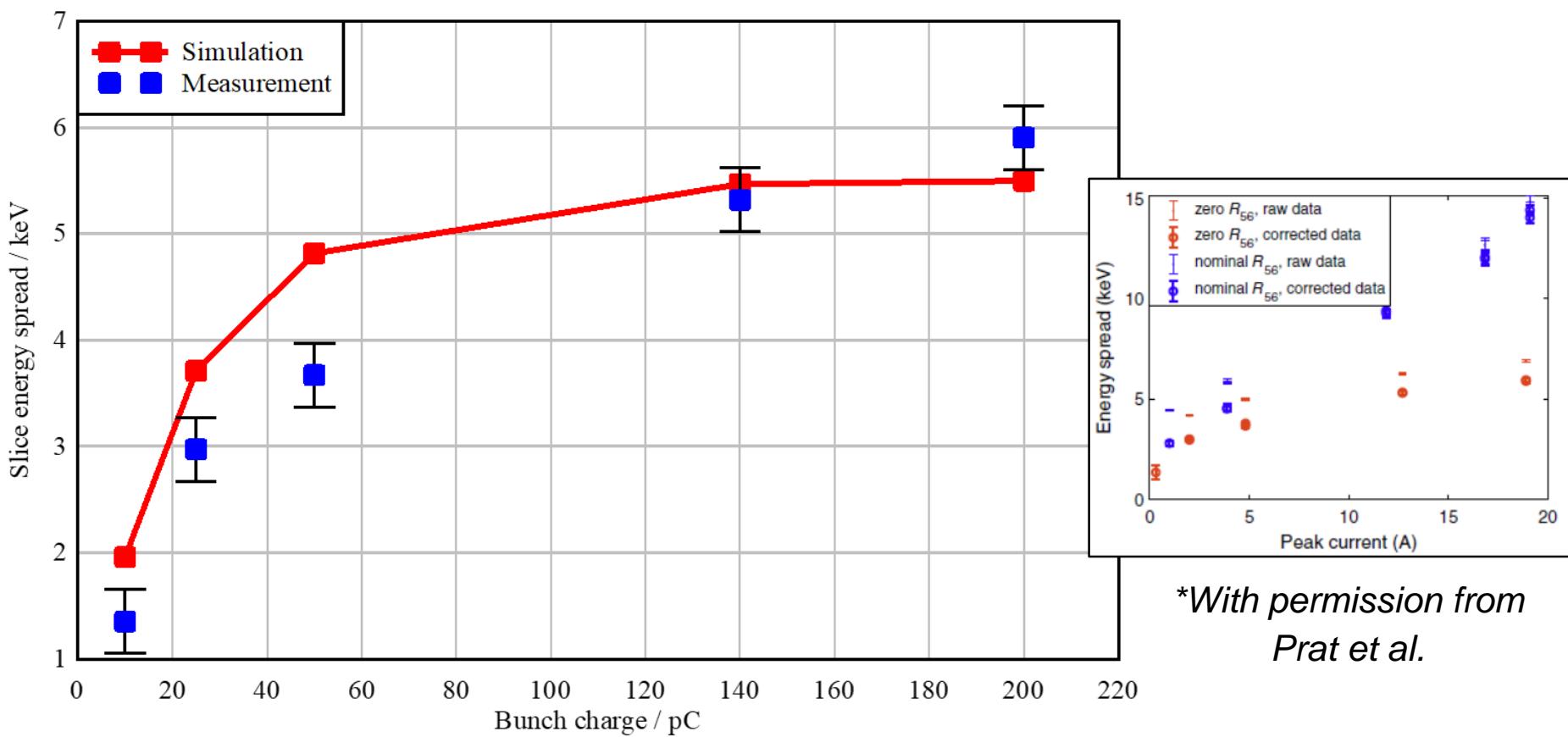
- Slice energy spread (“large” optics)



Simulations for the SwissFEL



- Charge scan

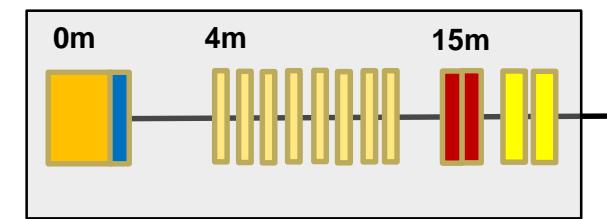


*With permission from
Prat et al.

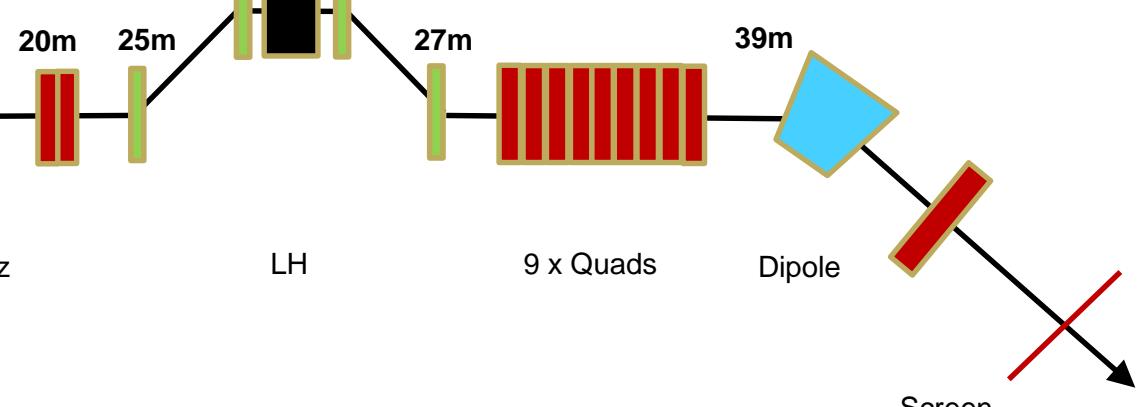
Simulations for the EuXFEL



The EuXFEL injector



Gun 1.3GHz A1 1.3GHz AH1 3.9GHz



- Final energy: ~130 MeV
- Bunch charge: 250 pC (nominal)
- 3rd harmonic AH1 switched off
- TDS structure (for the moment) ignored
- Energy spread measurement at the maximum energy slice

PHYSICAL REVIEW ACCELERATORS AND BEAMS 24, 064201 (2021)

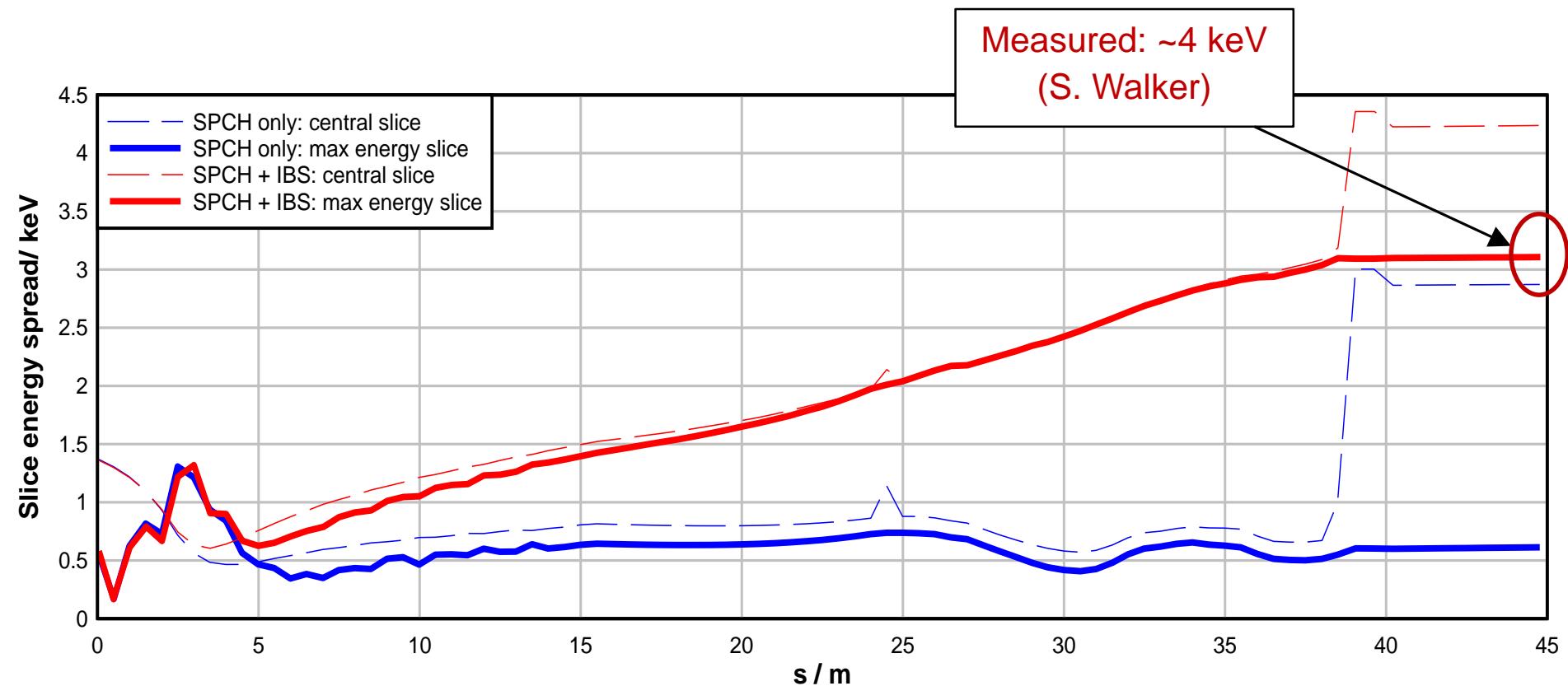
Accurate measurement of uncorrelated energy spread in electron beam

Sergey Tomin,* Igor Zagorodnov, Winfried Decking, Nina Golubeva, and Matthias Scholz
Deutsches Elektronen-Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany

(Received 19 March 2021; accepted 19 May 2021; published 2 June 2021)

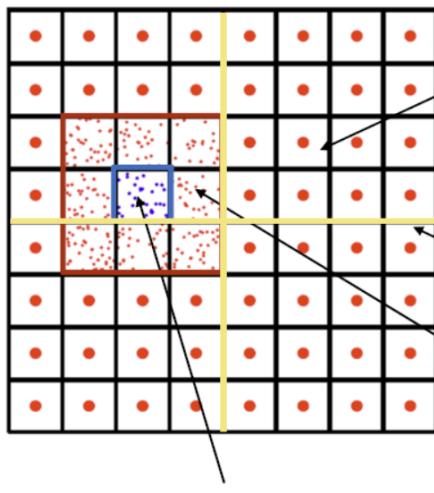
Simulations for the EuXFEL

- Slice energy spread calculations



Thank you very much
for your attention

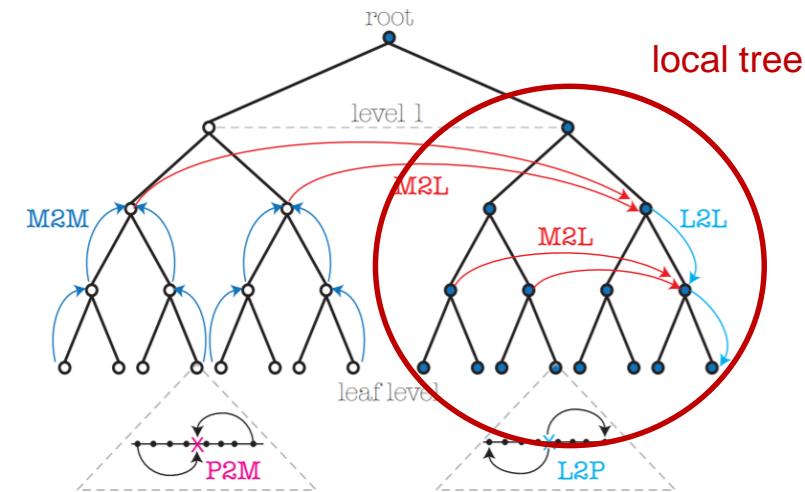
- The Particle-FMM solver



far neighbors – use multipole expansion in each box

domain boundary for parallel decomposition

near neighbors – apply P2P interaction



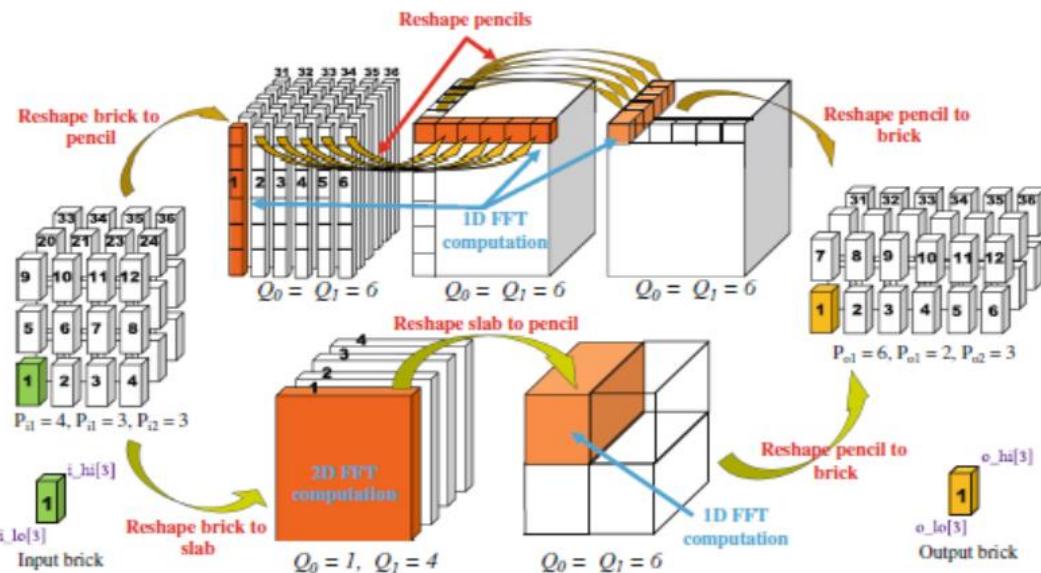
Hierarchic computation of mult. expansion
(Rokhlin & Greengard, 1987)

- Exponential expansions for M2L transformations -> reduce to $O(N)O(P^3)$
- MPI-parallelization using local tree decompositions
- Very efficient at high energies – noisy for space-charge dominated beams

The Reptil code



- The FFT-Green function solver
 - Uses Hockney's algorithm on doubled domains using IGF and shifted Green functions for the cathode charge
 - Using parallel 3D-FFT library – HeFFTe¹
 - Backend FFTW, Intel MKL (tbd. CuFFT)



Decomposition strategies for parallel FFT:

Input data is reshaped such that each processor performs a single 1D-FFT at a time¹

¹ A. Ayala, et al., “heFFTe: Highly Efficient FFT for Exascale”, (ICCS 2020)