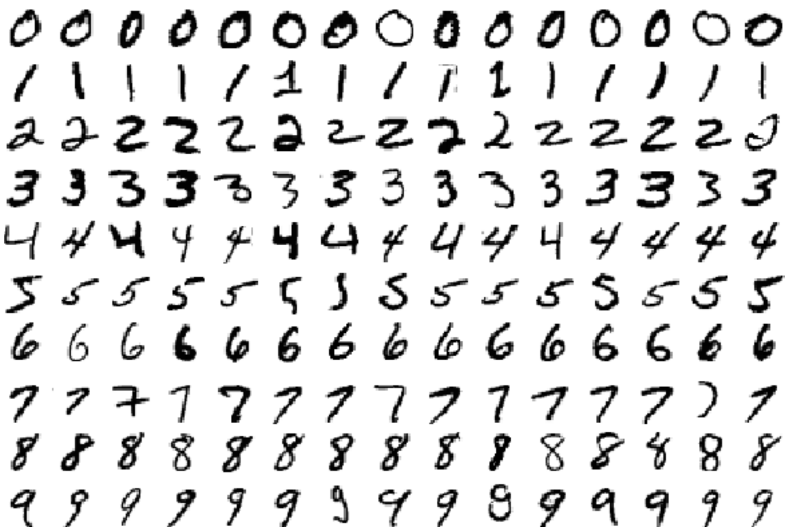
# Light source and FEL Simulations

Ilya Agapov, SLAC ML workshop, 1 March 2018

with material from
C. Fortmann-Grote, G. Geloni, S. Liu, S. Serkez, S. Tomin, I. Zagorodnov

# Motivation: understanding the application area of ML

- ML methods NOT covered in this talk. Rather try to define the problem(s)
- Focus of ML is on prediction-type problems
- Prerequisite: large training datasets (such as handwriting)
- Simulation use-cases for accelerators
  - Case 1.Train a model to reproduce a complex computation quickly
  - Case2. Use on-line data to train a model
- Fundamental limitation: for uncharted territory (novel schemes) physics knowledge is essential. We should hope to deal with computational complexity only
- Long way from Toy models to practical application

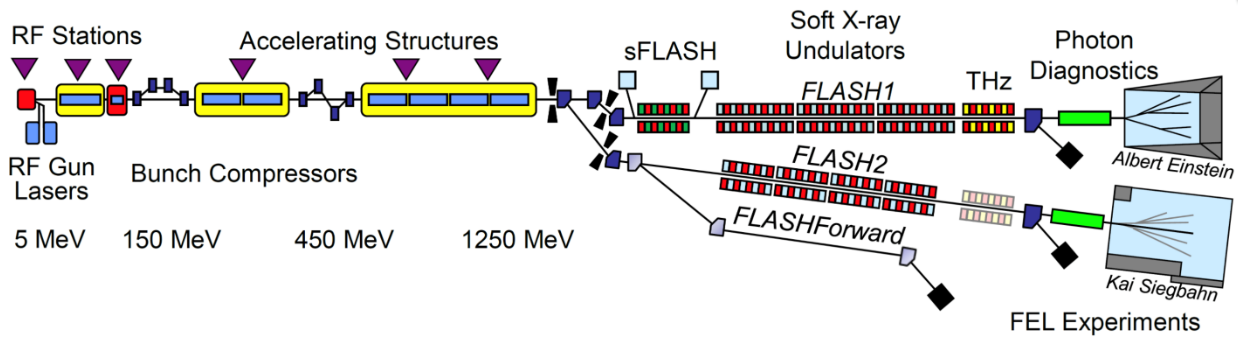


# Motivation: state of the art, conventional light source and FEL simulations

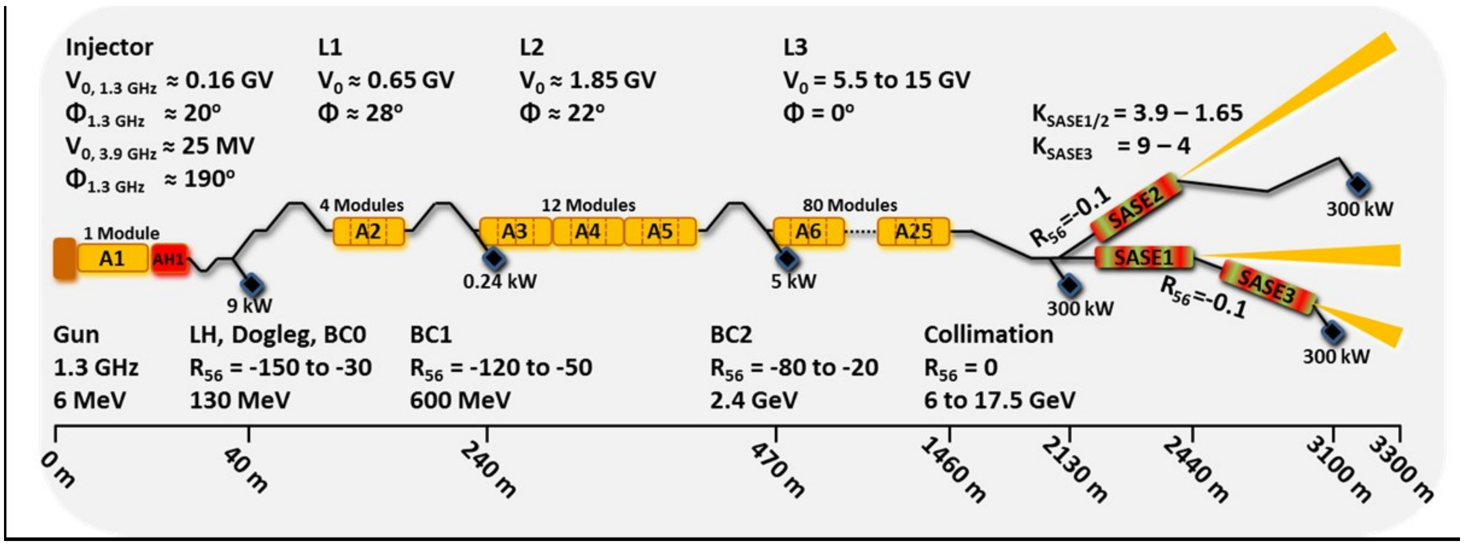
- In conventional accelerator facilities, very little unknown physics
- Following bottlenecks in the simulation are typical
  - Model (equations) well known, but the computation is expensive (linac collective effects, FEL, SR calculations)
  - Physics “well” known, but uncertainties in the model (complex systems)
    - Linac simulations (e.g. cavity models)
    - Precise optics modelling in a storage ring (< 1% BB accuracy)
- OCELOT on-line optimization project was started to address those issues (FEL simulations become too expensive to reproduce/optimize real machine with high precision)
- Another component: strengthening HPC platform at DESY (Maxwell cluster, 22472 cores but largely dedicated to on-line XFEL.EU experiments data processing, theory and PWA)
- Still another component: research into speeding up calculation methods
  - Parallelization, GPUs: fine, but only gets you so far, and code complexity an issue. Discontinued so far.
  - Empirical and simplified formulae (e.g. FEL estimator see later)
  - AI-inspired methods (limited progress – focus of this workshop, hope to boost)

# Overview of simulation needs: XFELs at DESY

FLASH

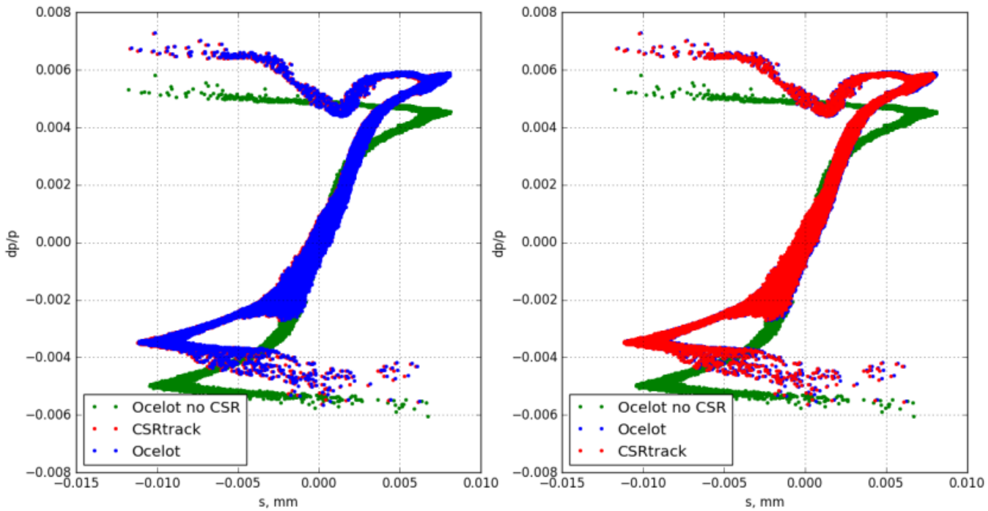



European XFEL



# Linac simulations: CSR

- Why would we need simulations after the design phase: understand what's going on, prepare for new generation (XFEL.EU CW upgrade, LCLS-II) and add-ons (self-seeding)
- Collective effect are essential for linac simulations
- Most important are
  - CSR
  - Space Charge
  - Wake fields

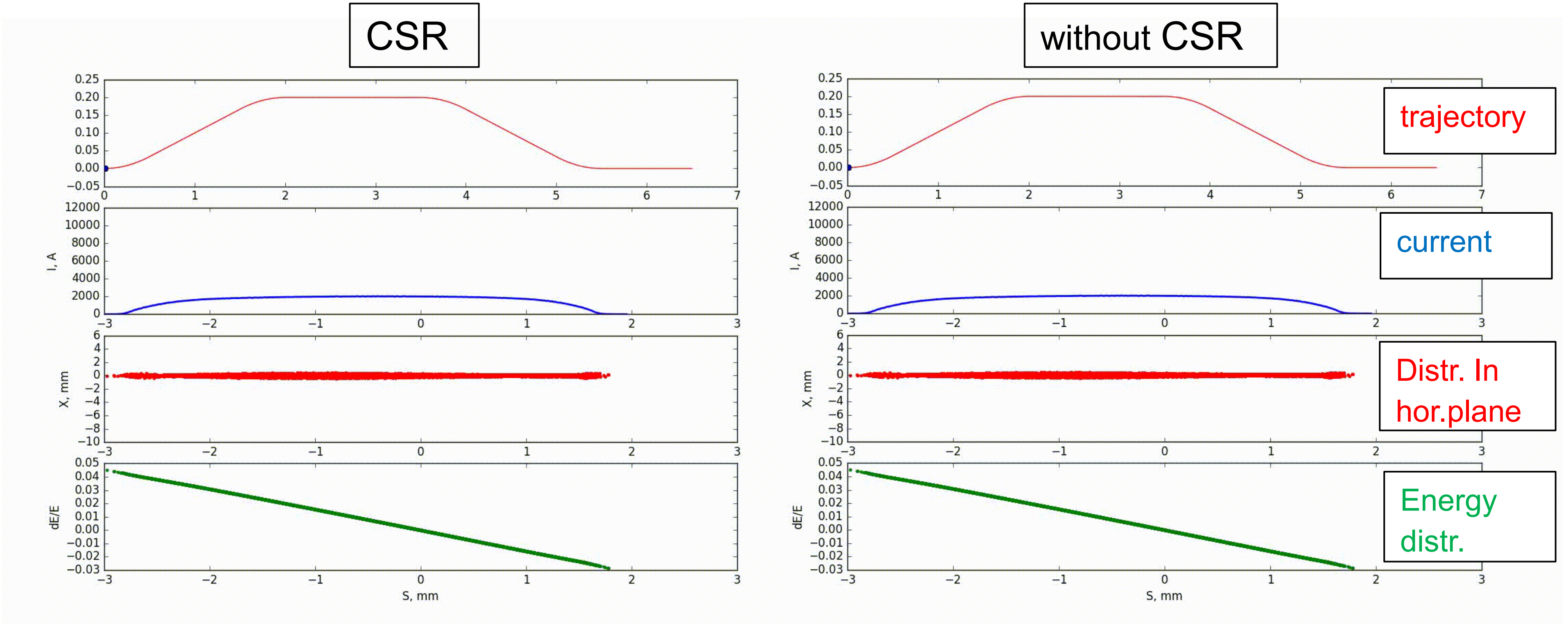



CSR. Cross-checking OCELOT vs CSRtrack. XFEL, BC2, Q=100 pC

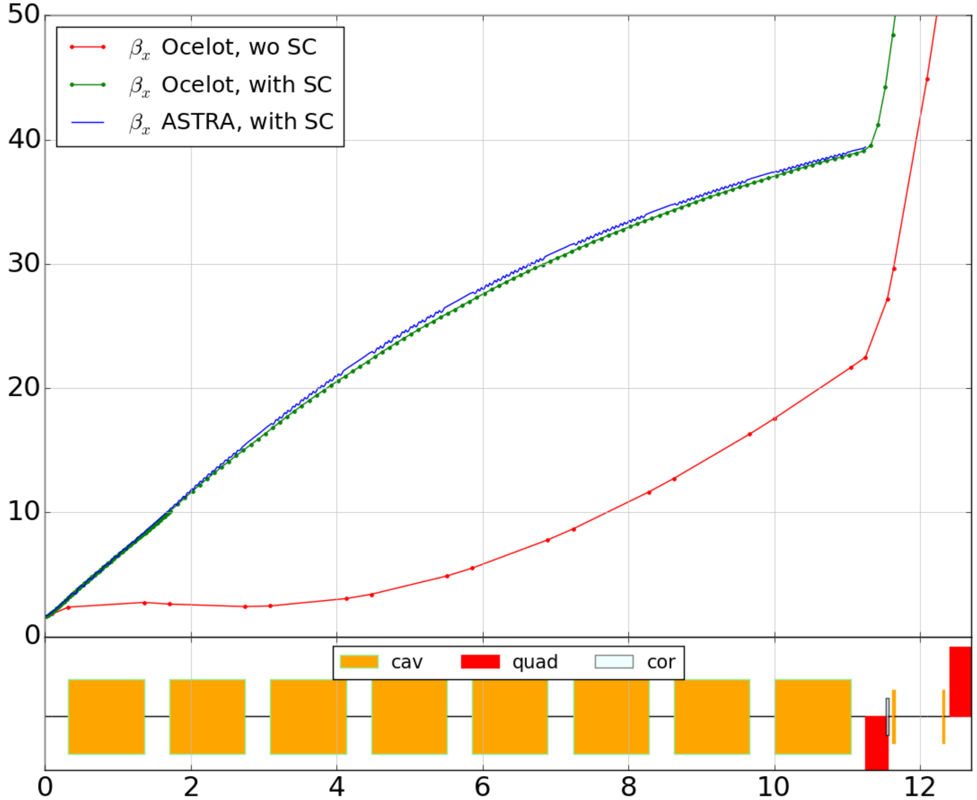
S.Tomin et al, OCELOT as a Framework for Beam Dynamics Simulations of X-Ray Sources, IPAC17, WEPAB031

Beam current was multiplied by **x100** to enhance CSR effect

Beam trajectory, beam current, spatial distribution (X), energy distribution



# Space charge effect + RF focusing cross-checking




<u>Energy:</u>

6.5 MeV – 154 MeV.

<u>Starting point:</u>

3.2 m from cathode

<u>Beam distribution:</u>

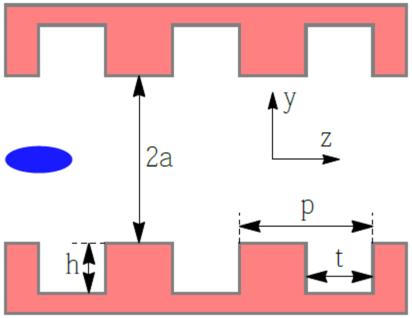
200 000 particles, Q = 250 pC

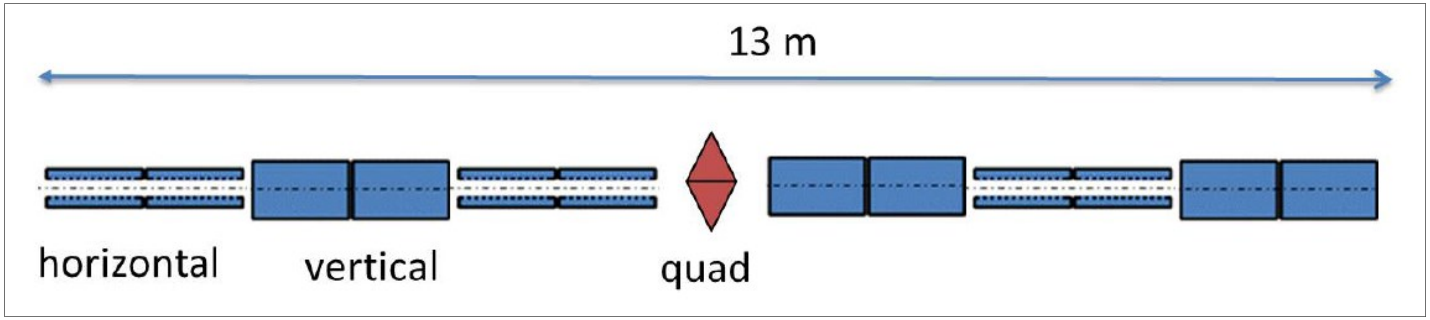
OCELOT: 2$^{nd}$ order matrices

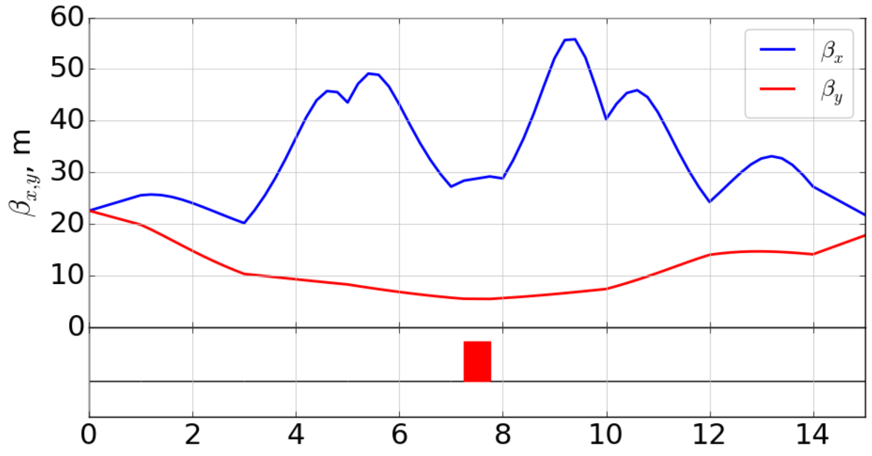
RF focusing:
Model of J.Rosenzweig and L. Serafini

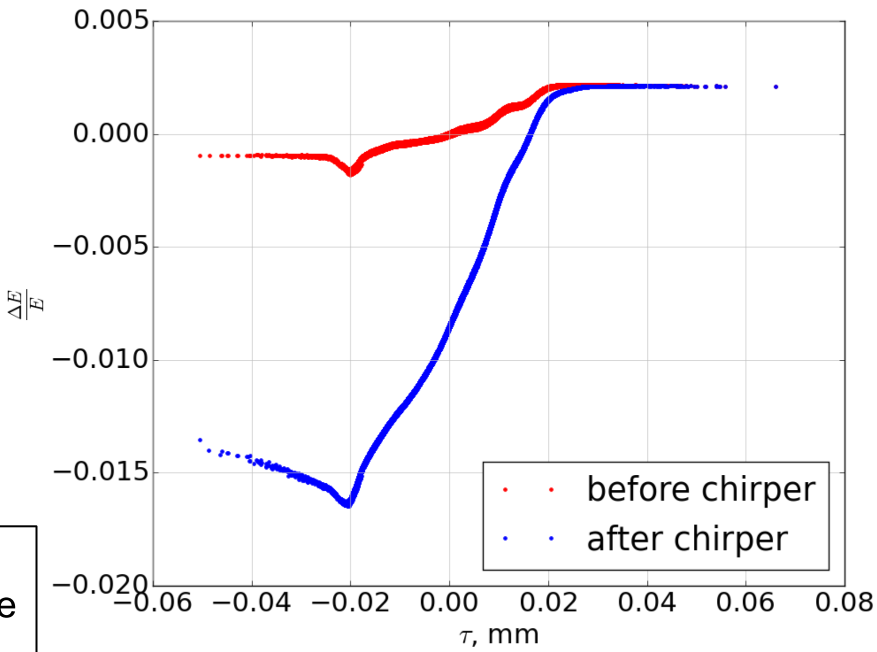
ASTRA: Runge-Kutta tracking in external fields

# Wakefield effects. Beam energy chirper.



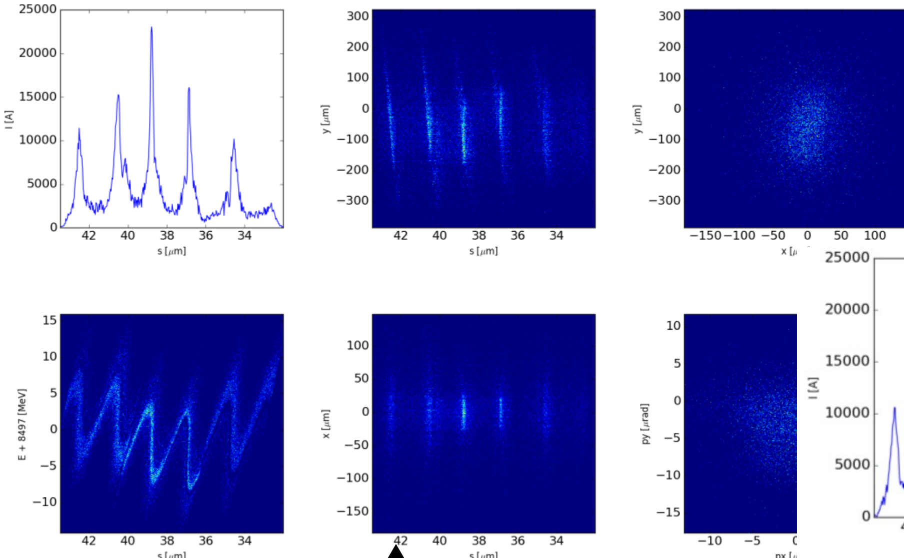



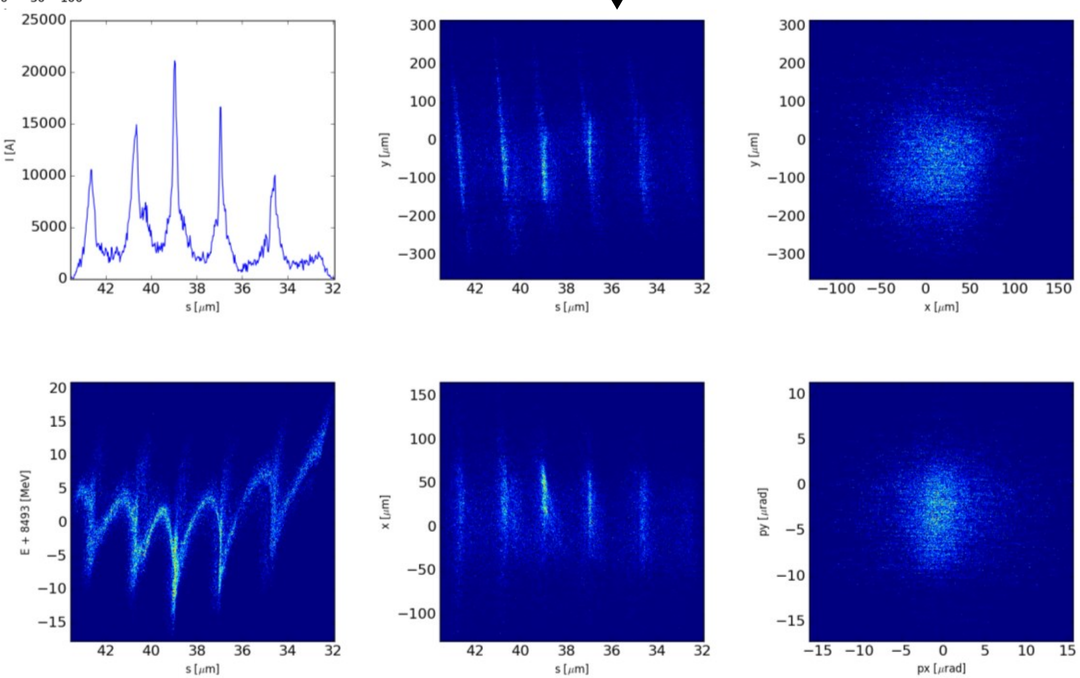




I. Zagorodnov, G. Feng, T. Limberg. Corrugated structure insertion for extending the SASE bandwidth up to 3% at the European XFEL.

- Simulations from an attosecond pulse study



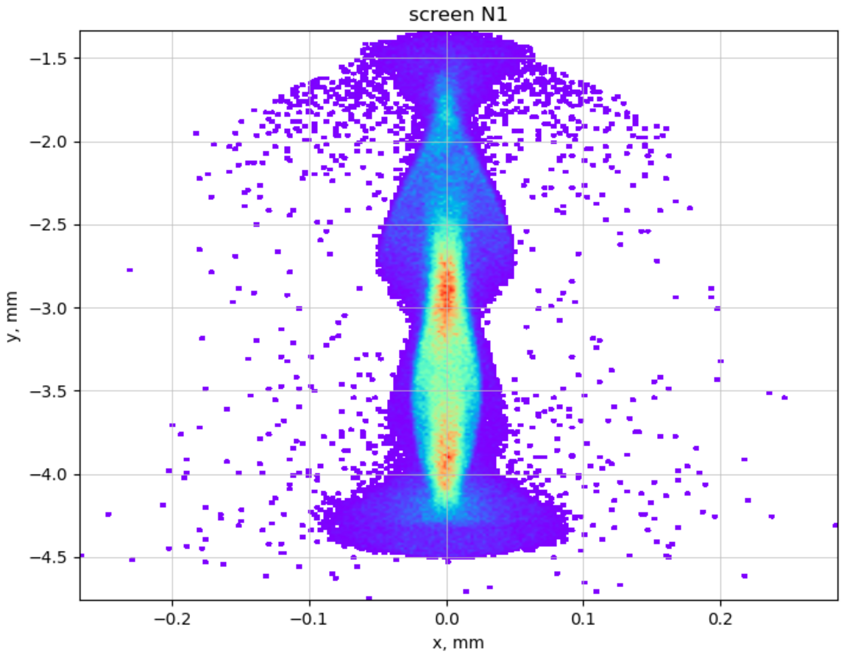

Tracking through chicane with CSR and 50 m long drift with SC



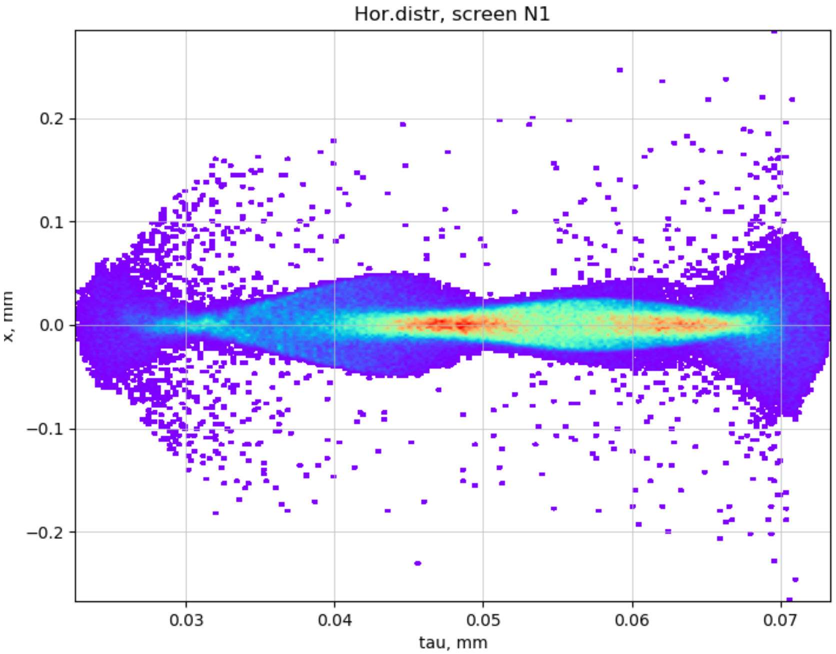

Tracking through chicane without CSR effect

# TDS simulation for European XFEL (OCELOT)

Image on a screen after TDS




Horizontal beam distribution at the position of the screen



# FEL Simulations

## New genesis4 adapter (beta version)

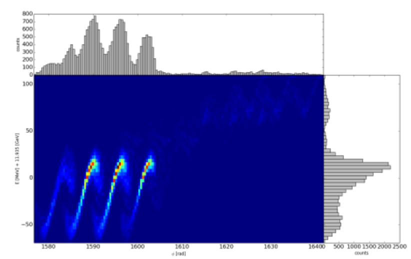
OCELOT ⟷ Genesis4$_{beta}$

ACSII input

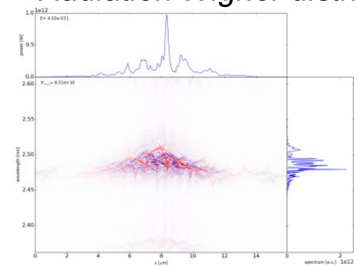
HDF5 output

Analysis

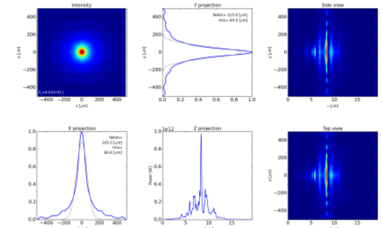
*Electron beam bunching*



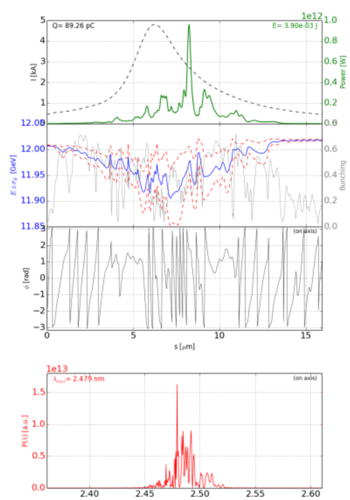
*Radiation Wigner distribution*



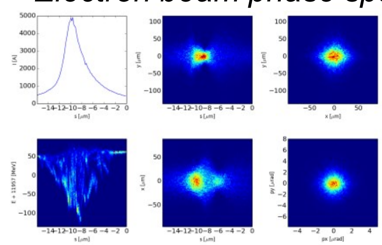
*Radiation projections*



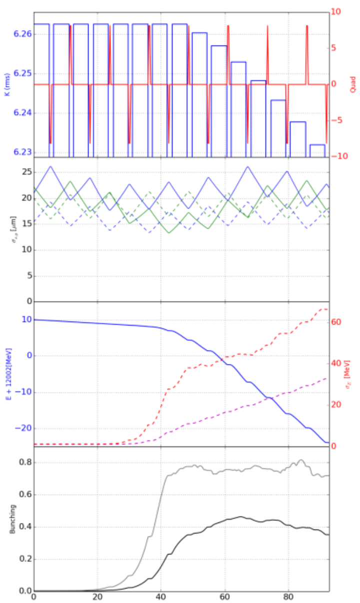
*Result along an undulator*



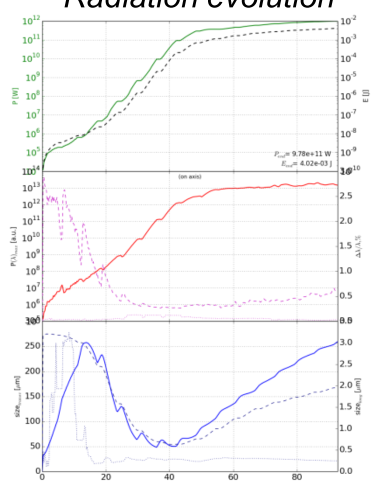
*Electron beam phase space*



*Electron beam evolution*

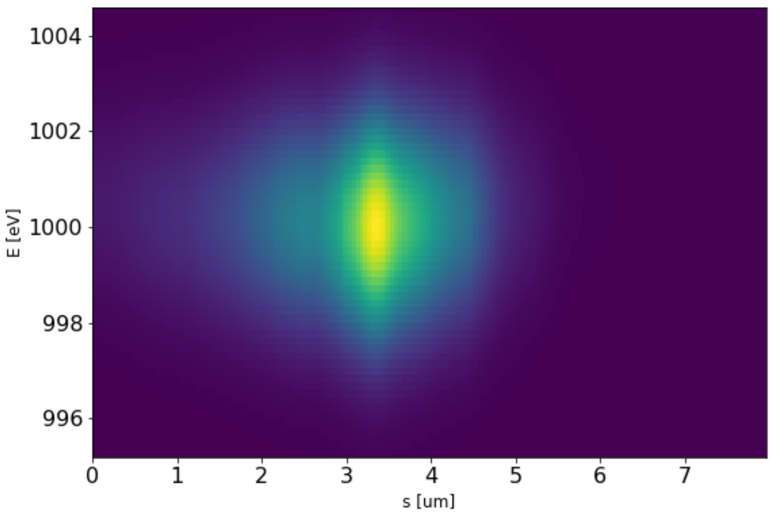


*Radiation evolution*

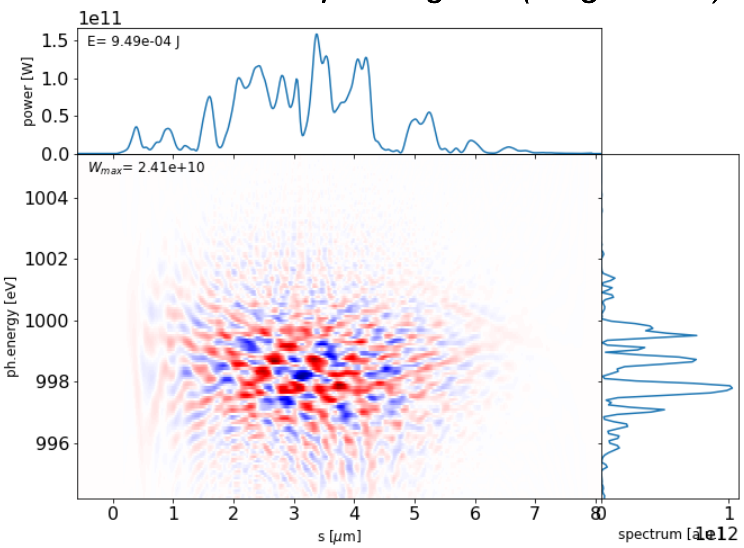


# Fast estimation of FEL performance (Ming Xie)

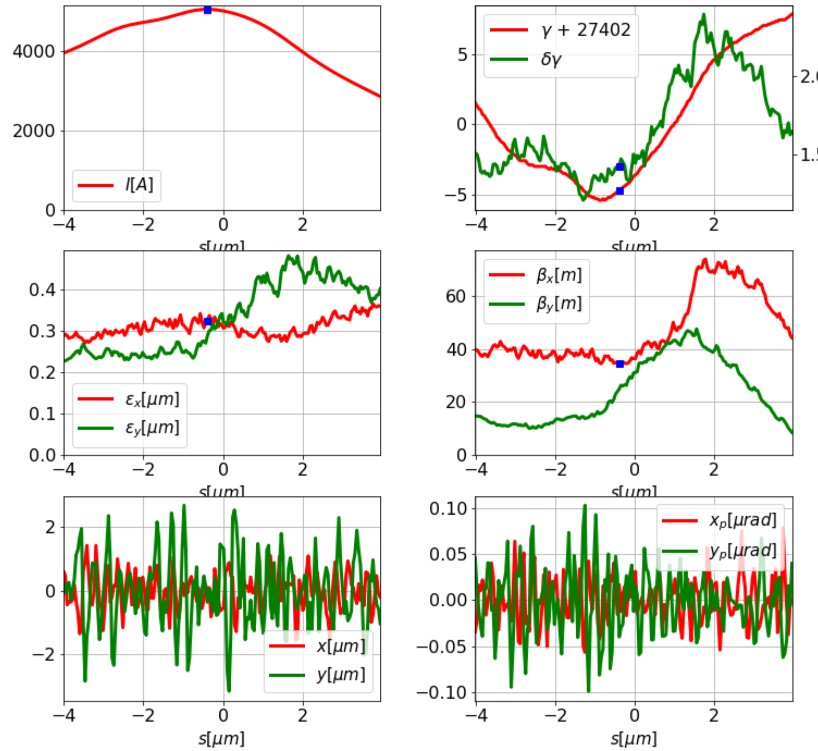
*Estimated spectrogram*



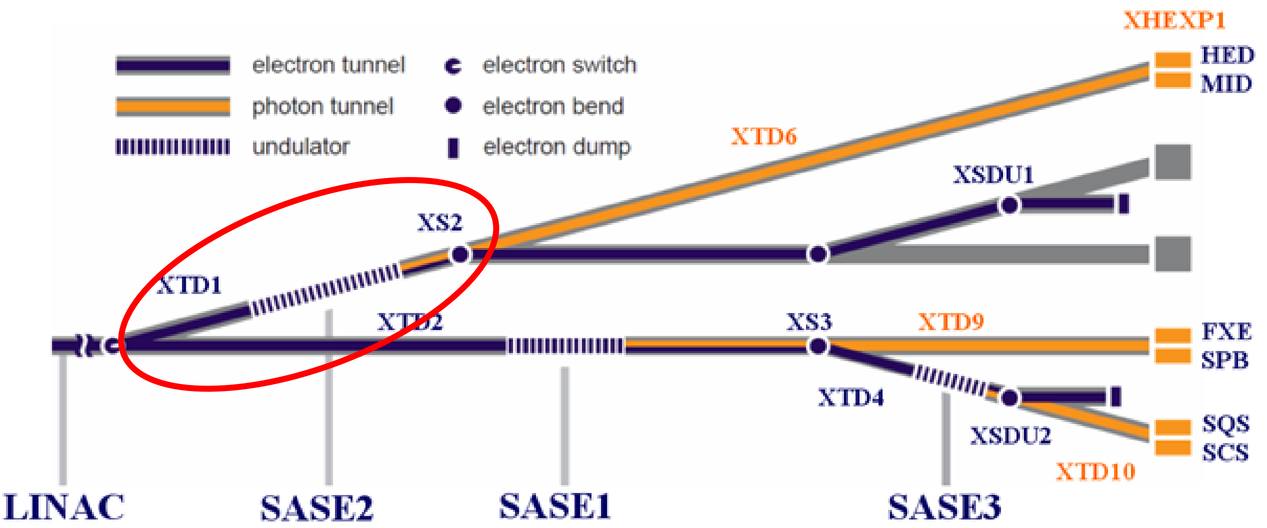

*Simulated spectrogram (single-shot)*




*Electron beam*



# Design and status – hard x-ray self seeding

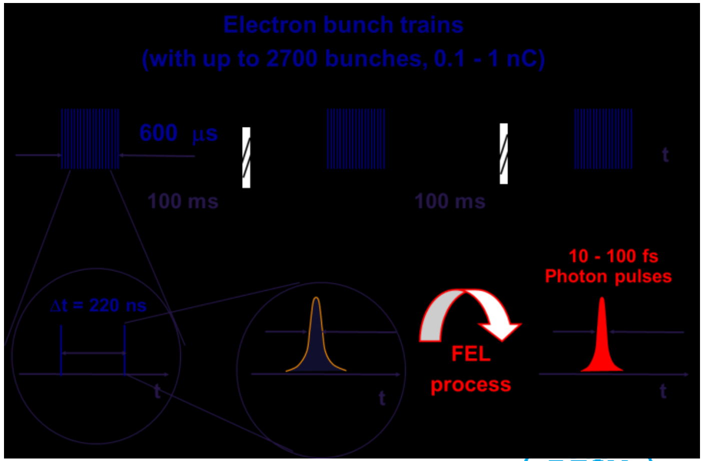



SASE2 line
(3 keV -25 keV)

→ to be first equipped with HXRSS

Specific for the European XFEL:

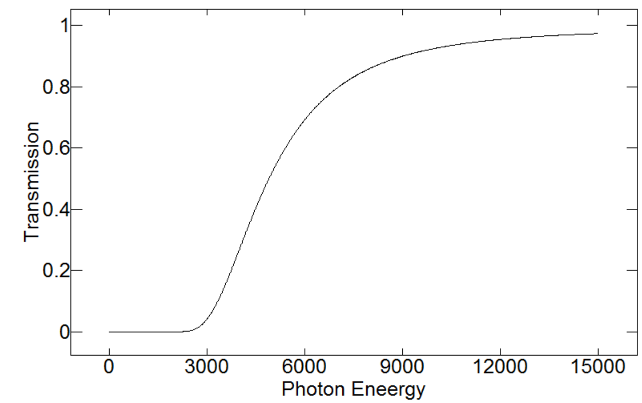
- High repetition-rate (FEL and SR heatload!)
- Long undulators (175m magnetic length at SASE2)



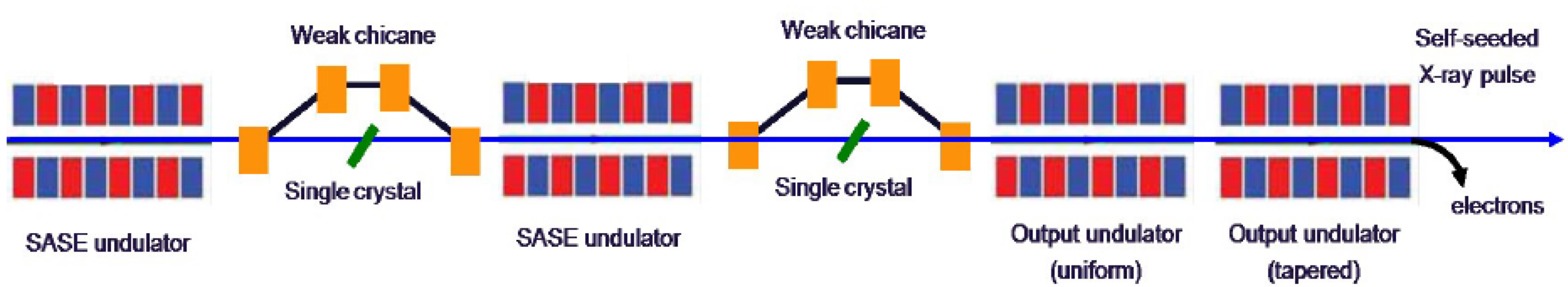
# Specific choices for the European XFEL

- Heat-loading from the seeded signals → depends on the fundamental
- Pulse heats up crystal locally → slow heat diffusion w.r.t. rep. rate
- local temperature increase → ω-shift beyond Darwin width (conservative) → Spectrum broadening
- Example: 100mum Diamond, C400; 3muJ incident at 8keV within the reflection bw in 1000 pulses;
- Conservative estimate: 0.7 μJ absorbed per pulse (…Realistic few μJ)

  →@8keV Deposited 24% → 3 μJ incident per pulse
  →@4keV Deposited 73% →1 μJ incident per pulse
  →@3.3keV Deposited 90% →0.8μJ incident per pulse

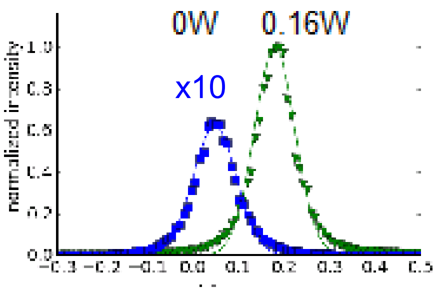



Heat-loading from seeded signals can be tackled with special 2-chicane design
At the second crystal, almost Fourier limited→ S/N gain: BW ratio SASE/seeded ~10



# Specific choices for the European XFEL

- Heat-loading from the spontaneous signal → basically independent of the fundamental
→ Broad spectrum

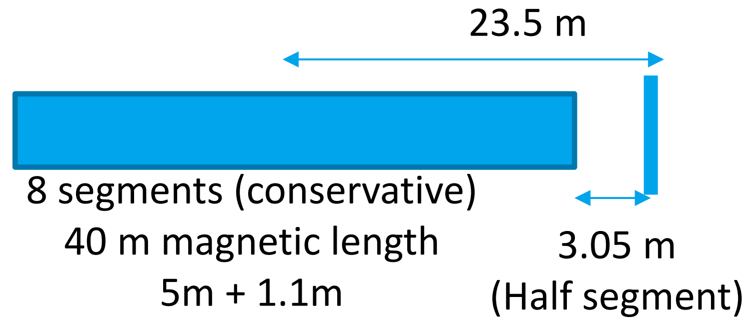



Si(440) analyzer crystal scans

X-ray reflection energy shift due to heat load
ΔE/E = 3.1 e-4

Experiment by L. Samoylova (European XFEL)

Spontaneous emission calculation:

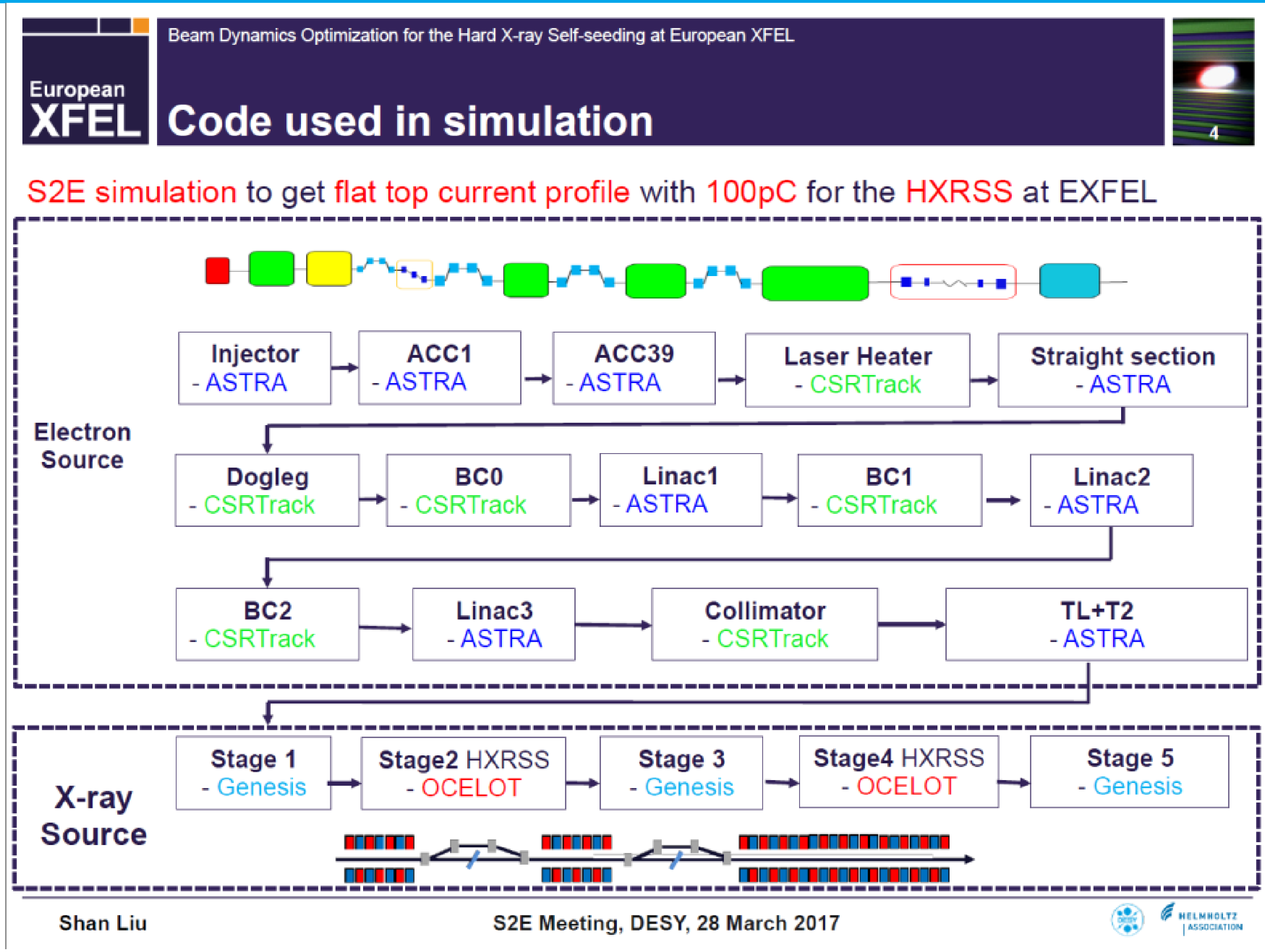



100 pC, 17.5 GeV, 8keV,100 μm thick diamond

| Deposited energy calculated using different methodes | 0-5keV | 5-37keV | 37-600keV | Total |
| --- | --- | --- | --- | --- |
| SPECTRA, [μJ] | 2.8 | 1.8 | ~1.5 | 6.1 |
| OCELOT+NIST, [μJ] | 1.67 | 3 | <0.8 | <5.47 |
| SPECTRA+GEANT4, [μJ] | 3.2 | 2.3 | 0.5 | 6 |

Total energy deposition: ~ 6 μJ

# HXRSS Simulations

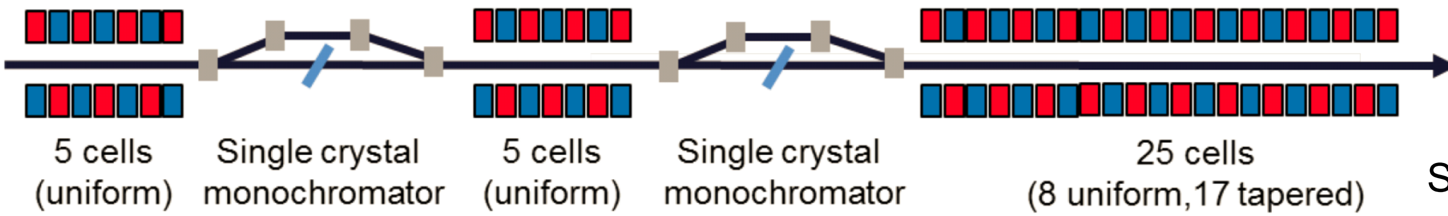



Now all the steps in the pipeline apart from the cathode can be done with OCELOT

# Simulations

## HXRSS application for

***Baseline SASE2 undulator (35 cells)***

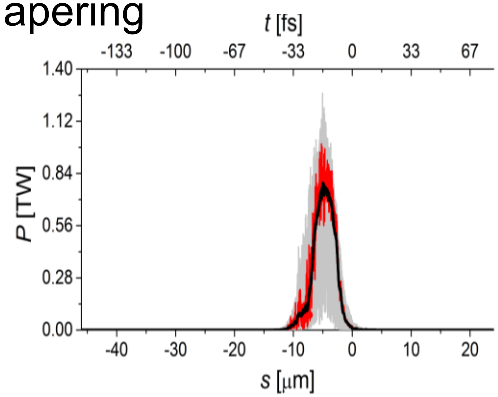


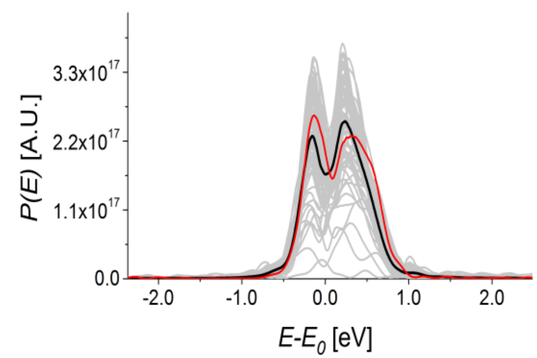

Application: Ultra-High Resolution Inelastic X-ray Scattering (UHRIXS)

Combination of high rep-rate HXRSS and Tapering

- Tapering: increases power
- HXRSS: decreases bandwidth
- Figure of merit for IXS: spectral flux

Standard mode of operation at 250pC




| | Intensity, [Ph/ pulse] | Photon pulse BW | Photon Flux, [Ph/s/meV] |
|---|---|---|---|
| w/o HXRSS | 7e11 | $\Delta\lambda/\lambda$~1.2e-3 or ~12eV | **1.5e12** |
| w/ HXRSS | 7e12 | $\Delta\lambda/\lambda$~1e-4 or ~940meV | **2.1e14** |

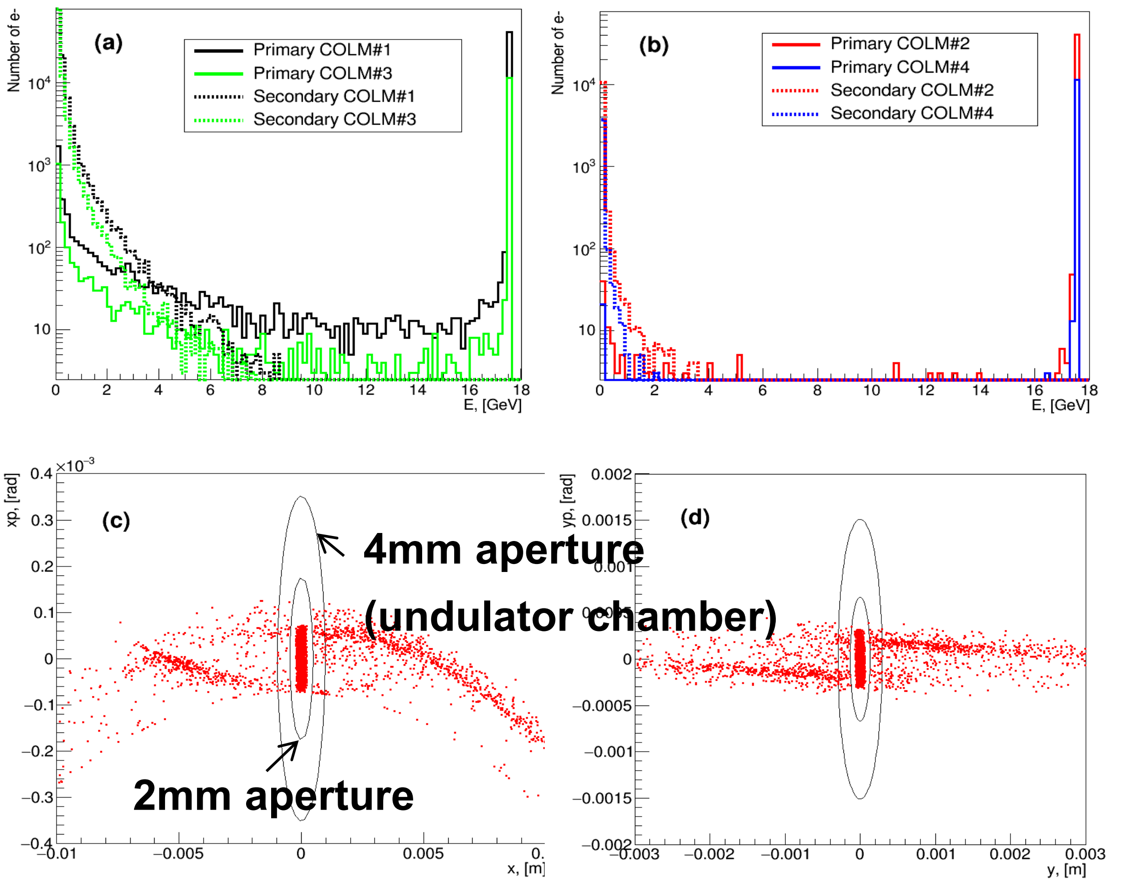
**O. Chubar, G. Geloni et al. J. Synchrotron Rad. 23 (2016)**

# Beam Halo Collimation Simulations (BDSIM)

- Energy distribution of the primary and secondary beam halo particles. Only those primary e-, which lost a small fraction of their energy (<1.5%), can reach the undulators.

- Phase space distributions at the end of the collimation section for the X (c) and Y (d) plane with $10^7$ input $e^-$. Electrons outside the dynamic aperture of the undulator chamber will be stopped at the undulator entrance. **The $e^-$ between the R=2 mm and R=4 mm apertures are those which may hit the crystal (assuming that the crystal is 2 mm away from the beam center).**

**S. Liu et al., in Proc. IPAC'17, paper WEPAB020**

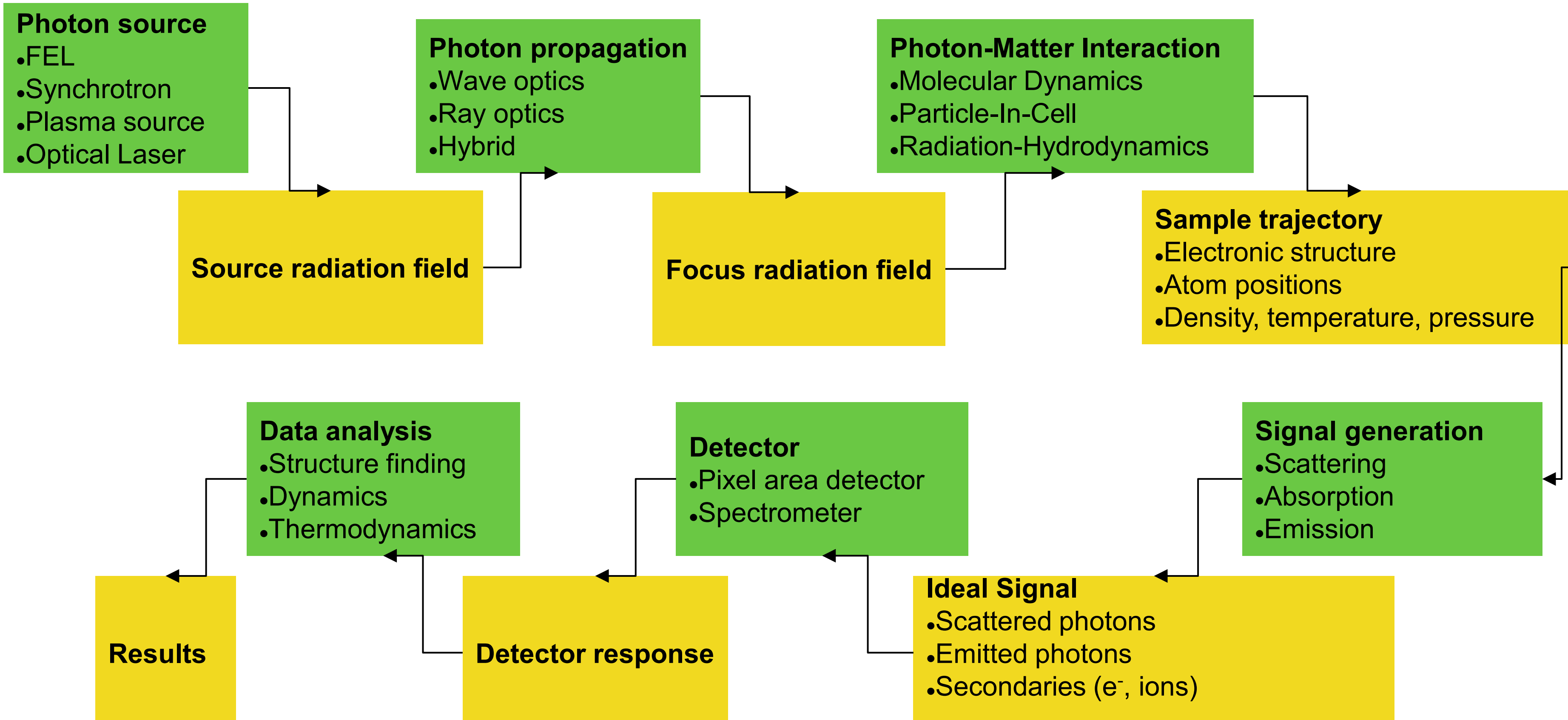



$N_{hits}$ is estimated to be 27±6 out of the total number of electrons $N_{total}=10^6$

**➔ $N_{hits} / N_{total} \approx 3\times10^{-5} < N_{critical} / N_{total} \approx 1\times10^{-4}$**

The crystal can be inserted up to a distance of **~2 mm** to the beam core **(~13 fs of minimum delay) !**

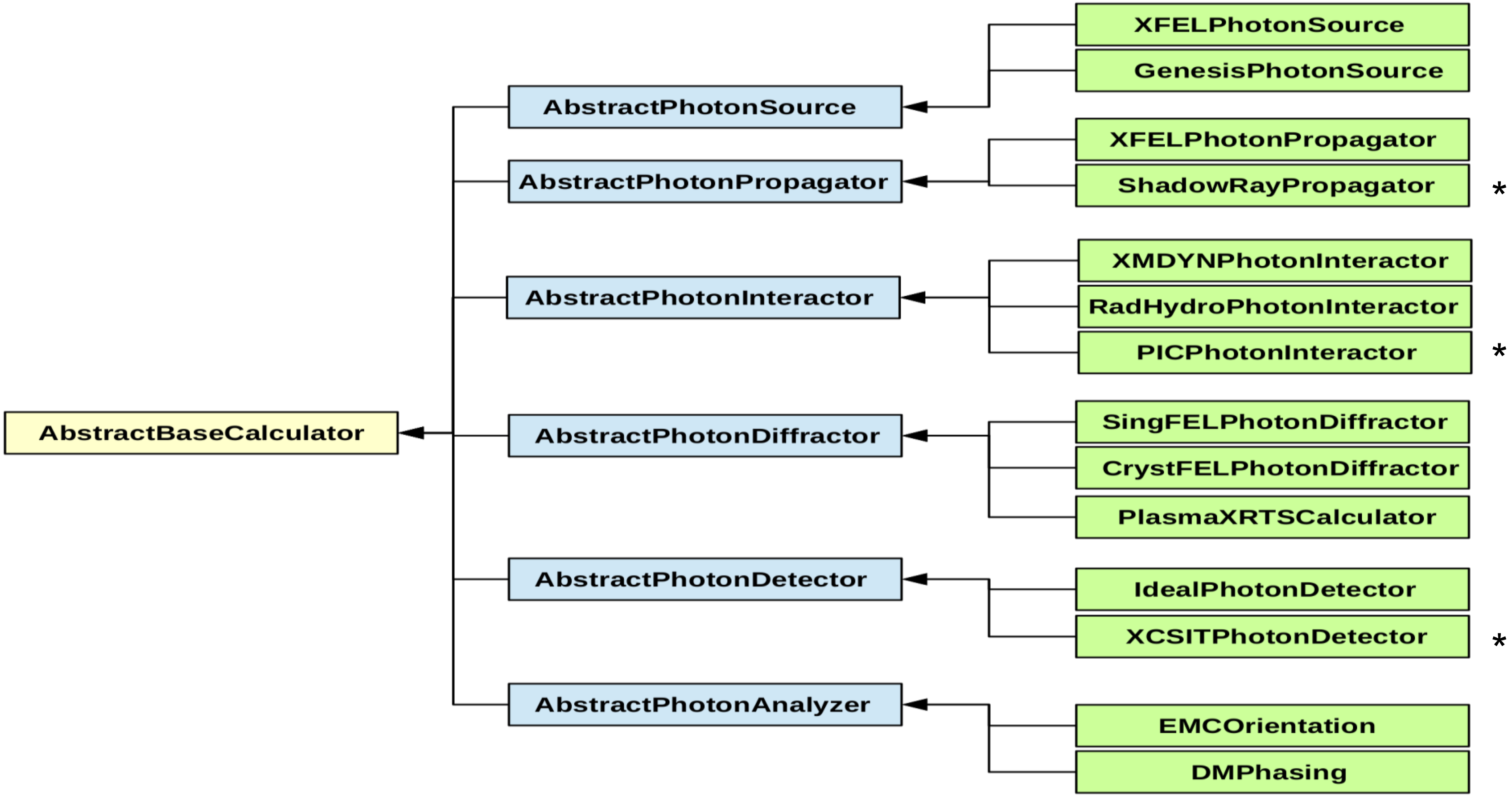
# SIMEX provides user interfaces and data formats for start-to-end photon experiment simulations




Calculators: Scriptable (python) interfaces to advanced simulation codes

Data interfaces using metadata standards

# SIMEX Calculators




* under development

# Bottleneck 1: Wavefront propagation

- Numerical propagation of time-dependent XFEL pulses
- Sampling: ca. 100X100 nodes in x,y, 100-1000 time slices
- Code: SRW with shared-memory concurrency (openMP)
- Wall time on 72 Intel 2.2 GHz CPUs: ca. 30-60 minutes per pulse
- S2E simulations require ~100 pulses to sample pulse fluctuations

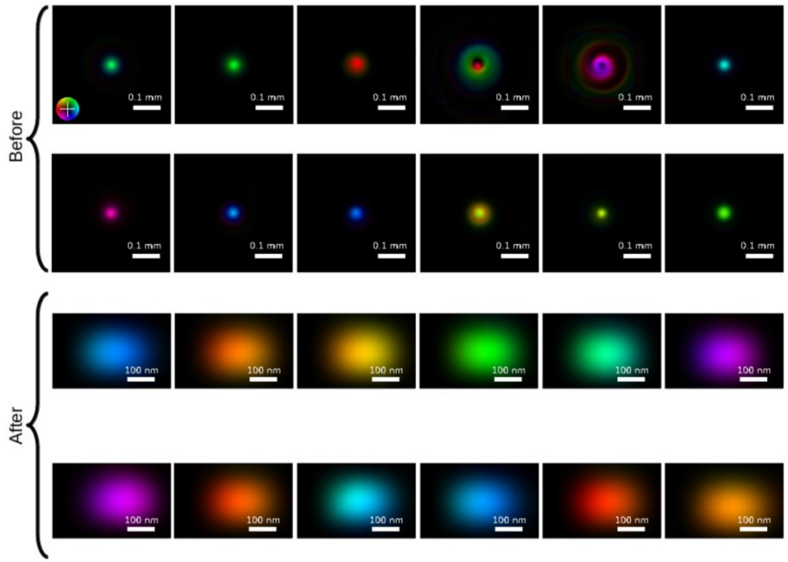



**Figure 6.** Intensity and phase maps of the SASE FEL X ray slices in a 9 fs pulse before and after propagating through the optics. The phase is color-coded. The distances between slices are about 0.2 fs.

Yoon et al. Scientific Reports **6** 24791 (2016)

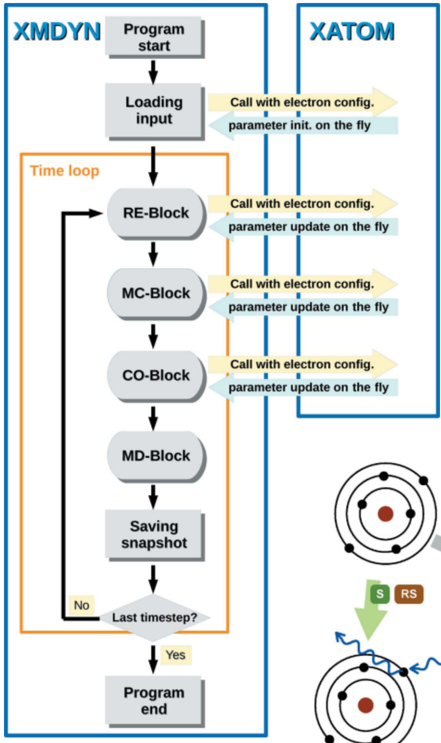
# Bottleneck 2: Radiation damage simulation

- Combined Hartree-Fock + Molecular Dynamics + Monte Carlo scheme to solve electron and ion dynamics in intense x-ray fields
- Code: XMDYN + XATOM, GPGPU enabled
- 1 Trajectory per GPU
- Small biomolecule (5000 atoms) runs for ~4 hrs, need ~1000 Trajectories
- Scaling (MD part) : ~$[N_{atom}]^2$
- → Large (realistic) molecules hardly feasible
- Alternatives: Continuum radiation damage models

Hau-Riege et al. PRE (2004) **69**, 051906

Jurek et al. J. Appl. Cryst. (2016)

Son et al. Phys. Rev. A **83**, 033402 (2011)



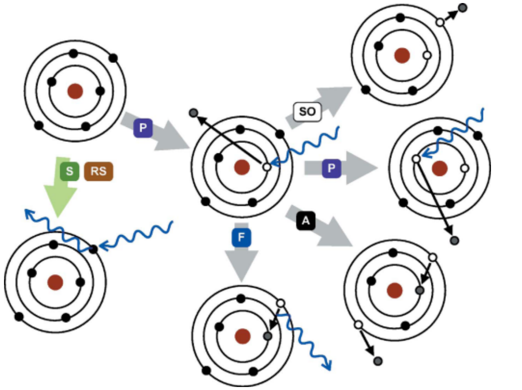

$$[-\tfrac{1}{2}\nabla^2 + V(\mathbf{r})]\psi(\mathbf{r}) = \varepsilon\psi(\mathbf{r})$$

$$V(\mathbf{r}) = -\frac{Z}{r} + \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3r' + V_x(\mathbf{r})$$

$$\rho(\mathbf{r}) = \sum_{i \in I} \psi_i^\dagger(\mathbf{r})\psi_i(\mathbf{r})$$

$$\frac{d}{dt}P_I(t) = \sum_{I' \neq I}^{\text{all config.}} [\Gamma_{I' \to I} P_{I'}(t) - \Gamma_{I \to I'} P_I(t)]$$

$$\Gamma_{I \to I'} = \frac{2\pi}{\hbar} |\langle \psi_{I'} | H_{\text{rad}} | \psi_I \rangle|^2$$

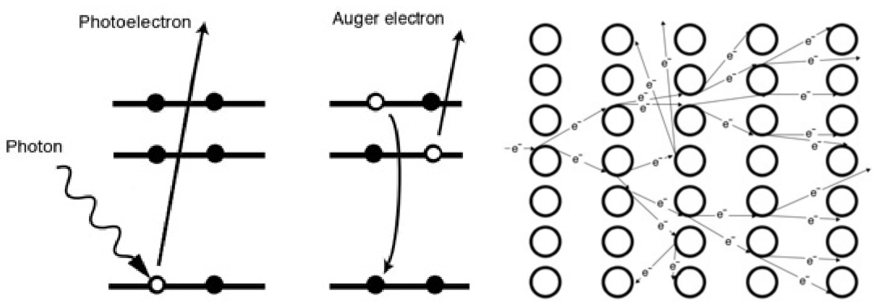


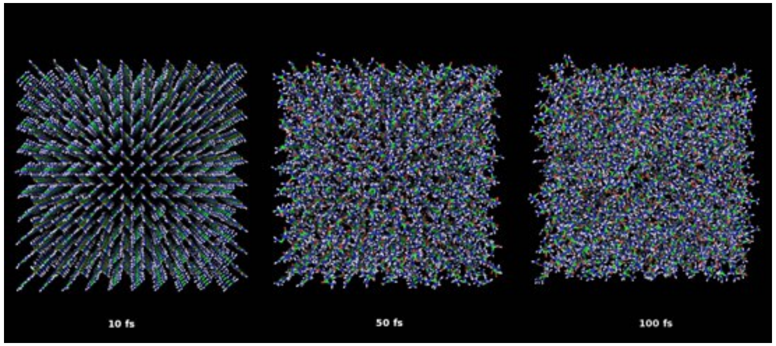
# Radiation damage processes and timescales

- SPI paradigm: Use ultra-short, intense x-ray pulses to diffract from single particles
- → Scatter enough photons despite small scattering cross-section and few scatterers
- → Probe before destruction

📖 Neutze et al. Nature (2000)

📖 desy.cfel.de/cid/research/understanding_the_physics_of_intense_x_ray_interactions/




0 1 10 100 fs

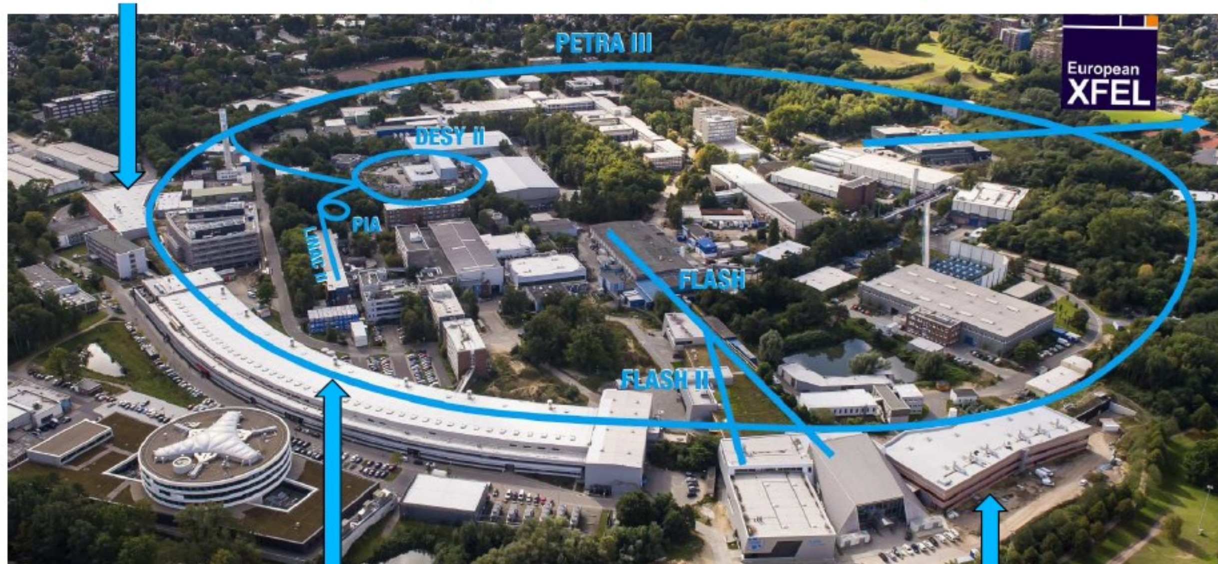
| Atom | $\tau_{Auger}$(fs) |
|---|---|
| C | 10.7 |
| N | 7.1 |
| O | 4.9 |
| S | 1.3 |
| P | 2.0 |

- Ultrashort pulses (few fs) may outrun secondary ionization and hydrodynamic expansion
- ↔ Short pulses contain less photon

# Storage rings

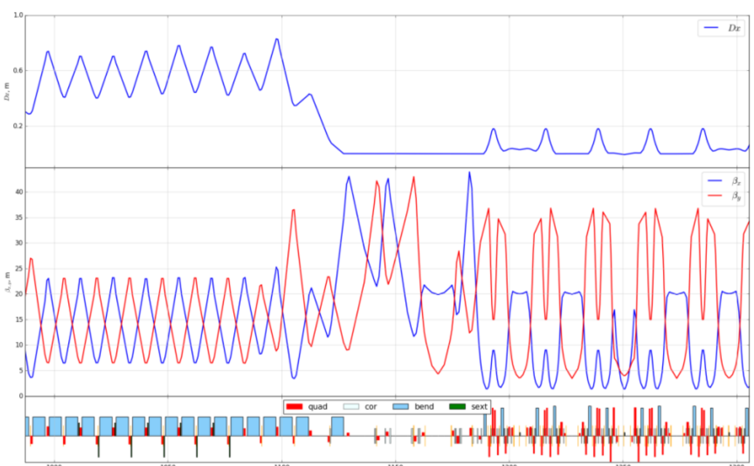
Third generation source
example Petra III

Extension Hall East
Ada Yonath 3 beam lines **(~ 3 free slots, status 2017)**



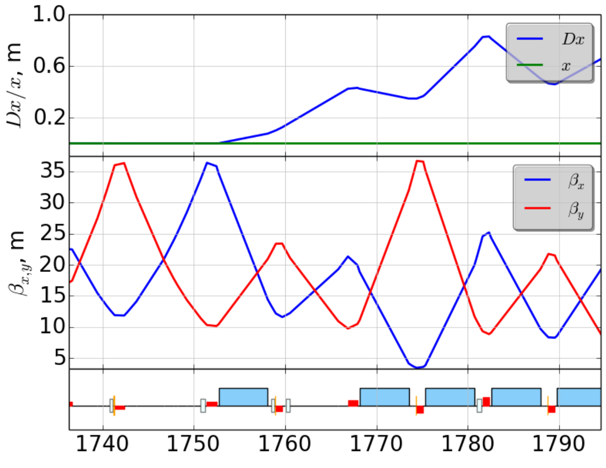

Max von Laue Hall
14 beam lines

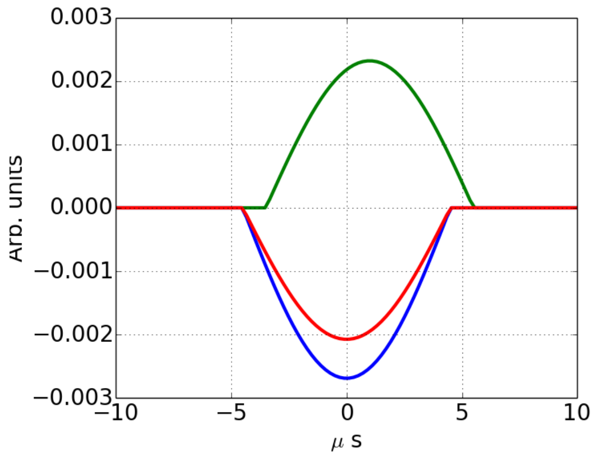
Extension Hall North
Paul P. Ewald
2 beam lines
**(3 free slots)**

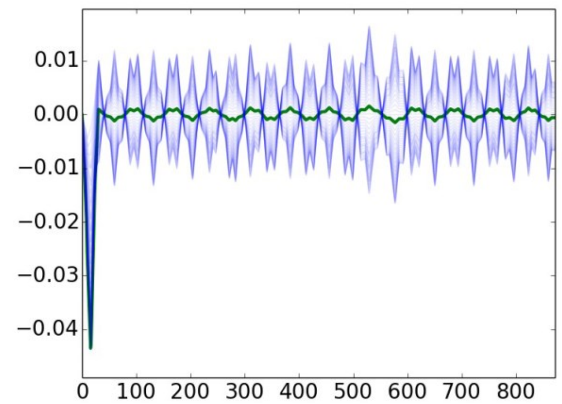


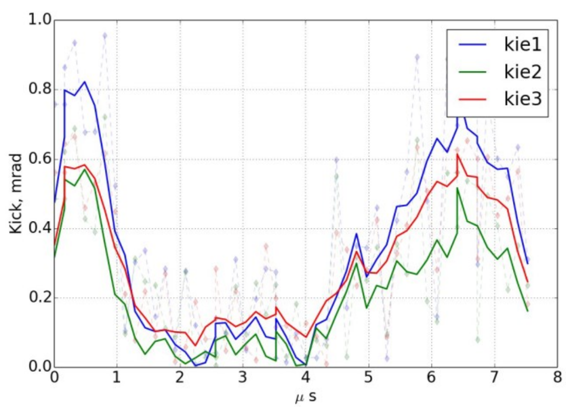

# Storage rings – typical example

Most non-technical work consists of optics/orbit correction, and transfer optimization
Typical example – orbit oscillations during top-up





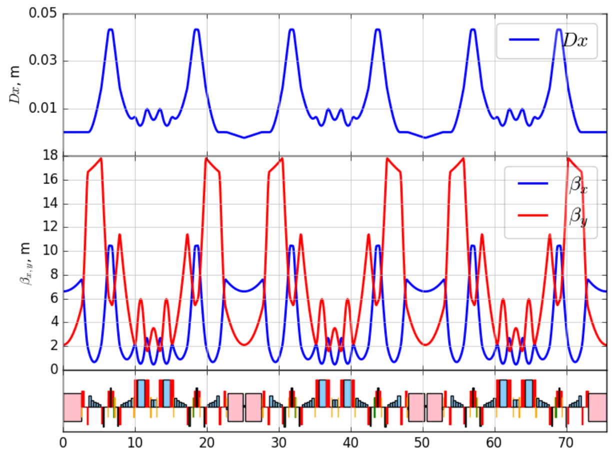

Fit with BPMs around the injection does not really work
Use empirical optimization instead

Similar situation with optics and orbit correction: starting from some precision we often don't know what's going on

But presently this is almost always ok with users

# Lattice design for MBA upgrade. PETRA-IV

Typical MBA lattice layout, also used at PETRA IV



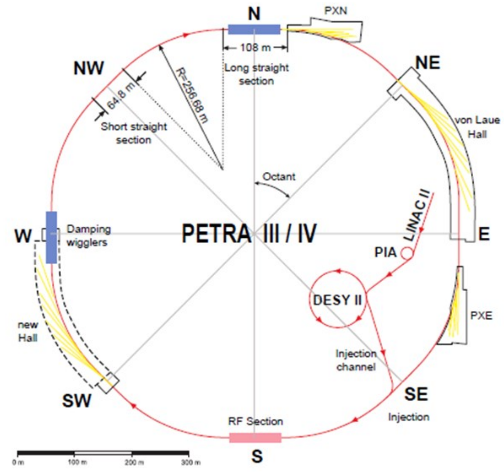
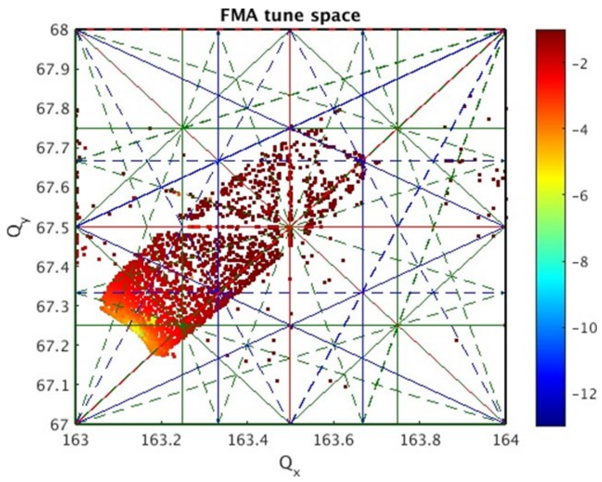
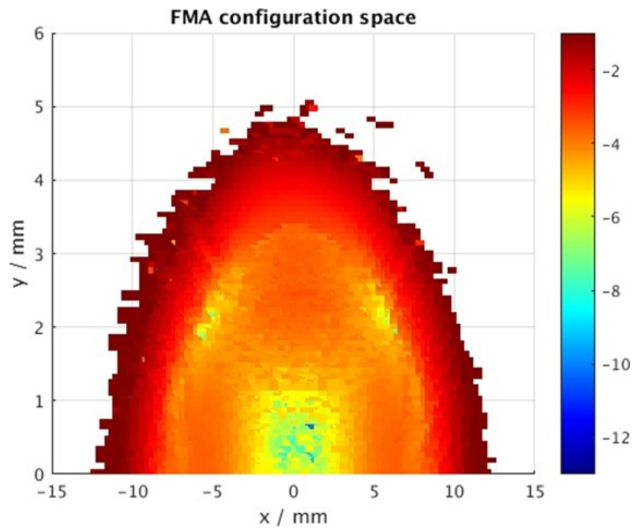



Figure of merit: DA



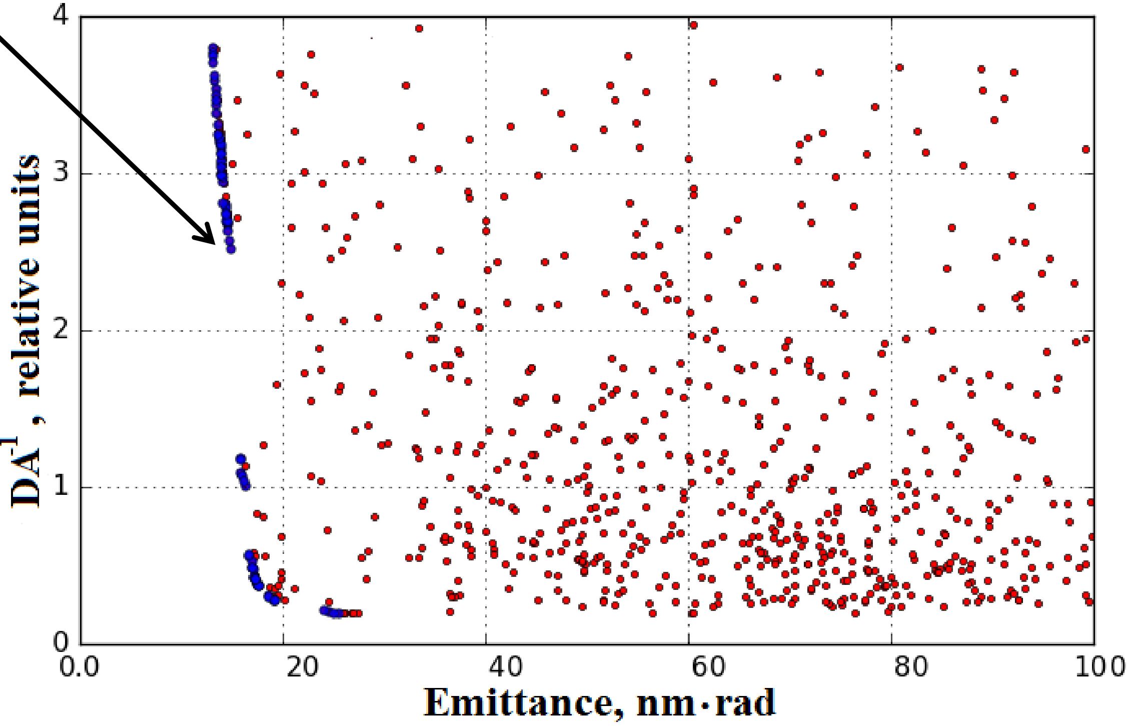
# Multi Objective Genetics Algorithm (NSGA-II)

Siberia-2 example

Pareto frontier

**Pareto efficiency**, or **Pareto optimality**, is a state of allocation of resources in which it is impossible to make any one individual better off without making at least one individual worse off

Dynamics aperture and horizontal emittance




**Objects: DA and horizontal emittance**
**Vars: 6 quadrupole families**

*E.Fomin, S.Tomin et al. Short Bunch Operation Mode Development at the Synchrotron Radiation Source Siberia-2, IPAC proceedings, 2016.*

# Can we use feature extraction to reduce calculation complexity? (speculation)

Fixing the bending, DA depends on

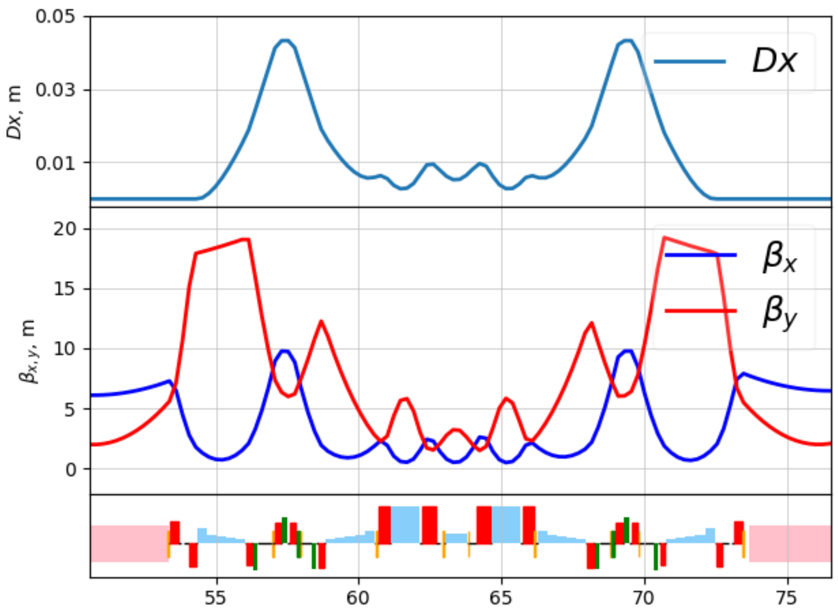
Type A features

Natural chromaticity
Sextupole strength
Phase advances between sextupoles
Phase advance of the cells
Phase advance of the octant
Machine tune
Machine natural chromaticity

N features (>17)

Type B features

Map coefficients (possibly in a Lie representation, or as resonance driving terms)
Up to 3rd or 4th order




Individual magnets: 12 per cell + matching sections

In a good design the number of individual Magnet circuits would be similar to the number of "features" to control

**We can't reduce the complexity**

# Misalignment studies (speculation)

But maybe we can speed things up

- Problem: predict DA for each possible alignment scenario

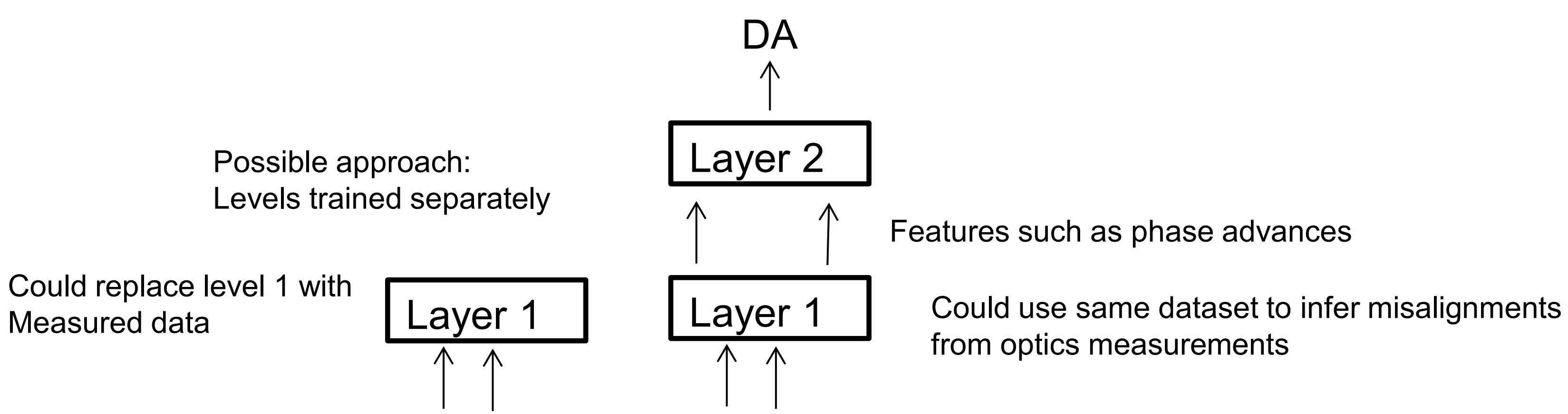
Simulation Procedure:  optics model with errors -> open trajectory, orbit and optics correction -> statistical calculation of DA
Very CPU consuming

- Possible approach:

Create large dataset of DA vs. statistical seed of individual magnet misalignments
Train NN to predict it
If NN generalizes well further calculations will be done instantaneously

Practical problem 1: We probably won't trust the NN result and will need to recompute in any case
Practical problem 2: Modifications to optics will invalidate the training set
Practical problem 3:Toy models are trivial (FODO), realistic model might turn out computationally infeasible

Possible advantage: HPC scalable and batchable



# What are the other feasible ML applications

- By definition ML cannot go beyond what’s in a training dataset.
- Feature selection in a (MOGA) optimization (simulation data mining)
- Speed up calculations in a long s2e chain chain (model training)
- Using NN as a universal fitting tool. Example: Storage ring brightness calculations. Analytical formulae for brightness are not universally accurate, need to resort to parameter scans with SRW/SPECTRA
- Speculation: if there is a standardized way to simulate everything with NN, possibility of creating complex models by connecting such components can emerge

# Conclusion outlook

- Many sophisticated simulation tools are in place for (conventional) light source and FEL facilities
- Calculation speed and setup uncertainty is often an issue
- ML methods have potential in
  - Speeding up calculations in a long s2e chain
  - Combining measurements and simulations by replacing NN layers with measured data to build better models

- This is all still highly speculative for realistic applications
- A universal problem: generating useful datasets is not cheap

- Long way from toy models to practical problems. We need a “benchmark” that is hard enough to show feasibility (netflix challenge, DARPA grand challenge,…)

- Some simulation tasks covered here can be considered such benchmarks

- Real benefit will probably appear when AI/ML techniques are used widely in a standardized way (exchange neural networks instead of madx files)

- Lots of infrastructure work is to be done in parallel (DAQ, interface standardization, etc. )