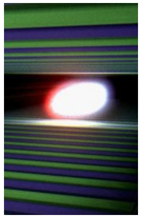
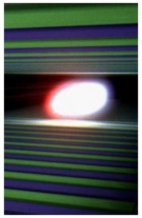


Multiphysics simulations of beam dynamics, synchrotron and free electron laser radiation.

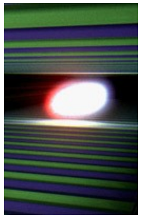
I. Agapov, G. Geloni, S. Tomin

Contents



Contents:

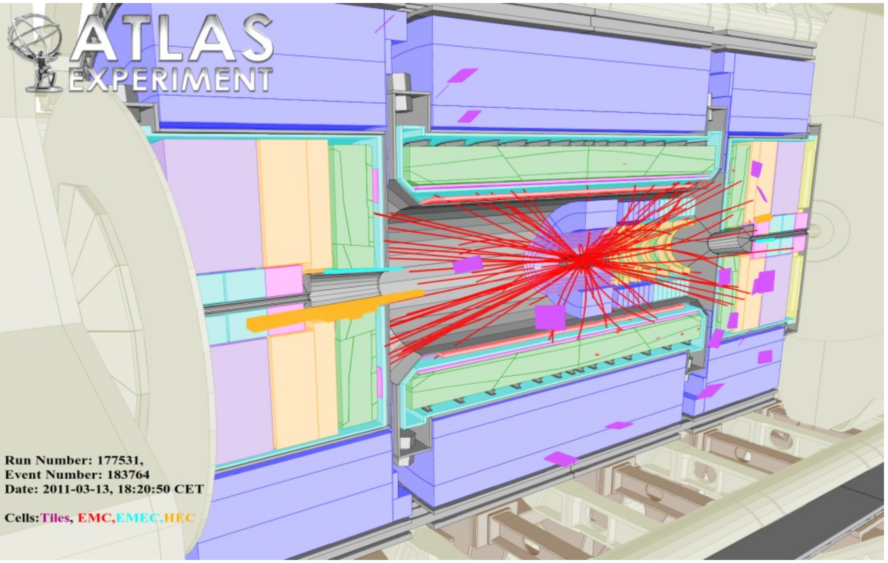
- Xcode/xframework
- Radiation properties at the European XFEL
- Nonlinear dynamics studies in synchrotrons
- Longitudinal insertion for short bunches or lasing in a storage ring



I/IV
Xframework

Xcode/xframework

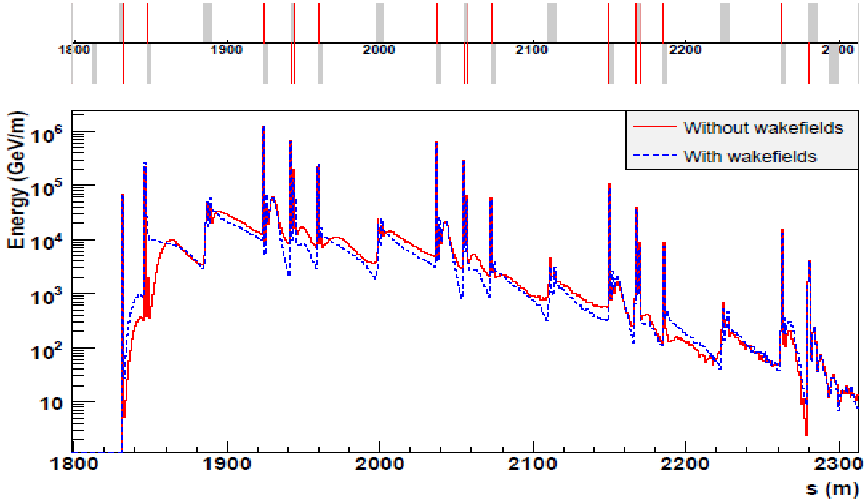
- 'xframework' refers to the common framework + integrated modules, the distribution including 3rd part codes (srw, genesis) is referred to as 'xcode'
- Open source https://code.google.com/p/xfel-xcode/
- SVN, unit tests, otherwise 'agile development'
- 2Yr in development
- Inspired by HEP software (Geant4) and OpenFOAM. Addressing such issues as:



- Simple and extensible geometry description . (MAD not extensible, XML or other cad-level options not simple)
- Scripting
- Modular physics
- Seamless embedding into on-line tools

Multiphysics simulations

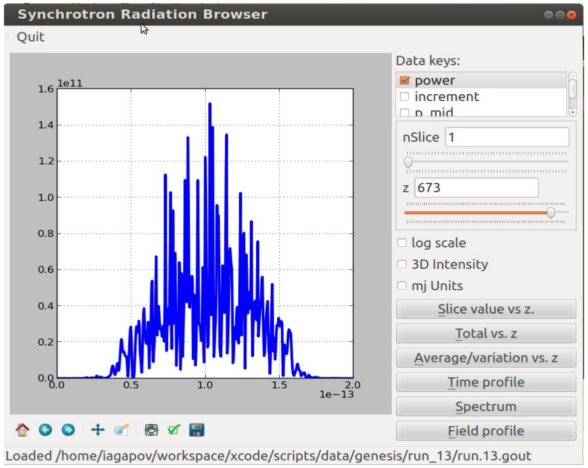
- One common example of a 'multiphysics' problem in accelerators – collimation
- CLIC Beam Delivery collimation: Wakefields + secondaries (BDSIM/PLACET)
- XFEL needs: FEL, SR, space charge, CSR, wakefields, etc....
- Always reinventing protocols to exchange data between codes; different physics can be included only iteratively, not on small time steps
- Open python library can provide much simpler solution to the problem



From Tracking Studies of CLIC
Collimation system
Agapov et al PRST-AB (2009)
Wakefields calculated with GdFidl, beam core tracked with
PLACET and the halo with BDSIM. In this case wakefields
Have negligible effect.

FEL simulations

- Genesis is now an 'industry standard' FEL code
- Automatically generating genesis input from standard xframework decks, easy controls of run parameters
- Postprocessing tools for genesis: I/O and statistical analysis
- 1D python fel model
- Optimization routines and parameter scans (python)
- Work on integration of other solvers in progress (ALICE c/o I. Zagorodnov)



Data keys:
☑ power
☐ increment
☐ p_mid

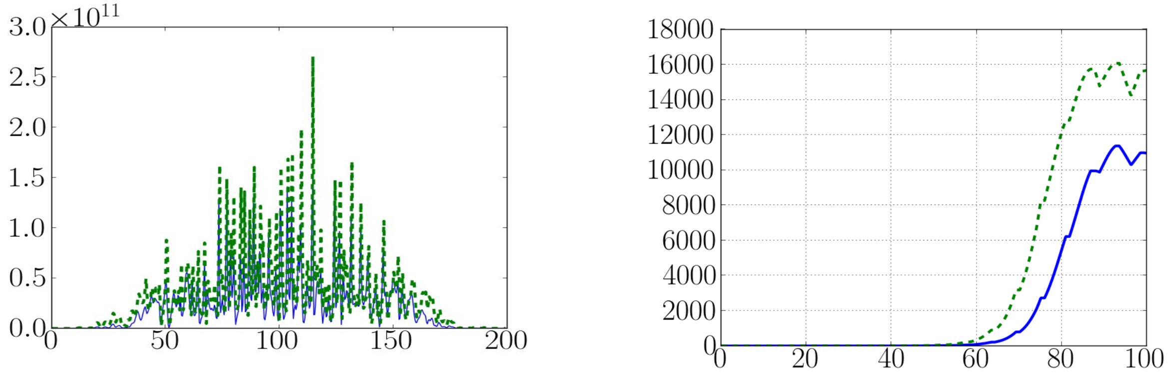
nSlice 1

z 673

☐ log scale
☐ 3D Intensity
☐ mj Units

Loaded /home/iagapov/workspace/xcode/scripts/data/genesis/run_13/run.13.gout

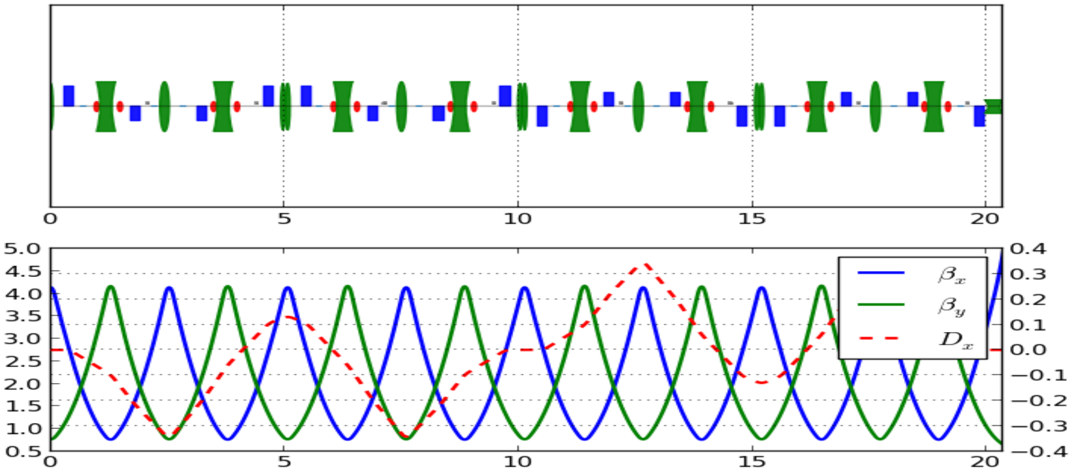
Radiation parameters of SASE3, with postprocessing GUI (left)



Beam optics

- Completely embeddable and extensible e optics module – not an optics code
- Standard optics calculations included in distribution as scripts
- Embeddable: call from any python code
- Extensible: user can define new elements, redefine transfer maps and attach
- any additional features to beam elements w/o changing the module

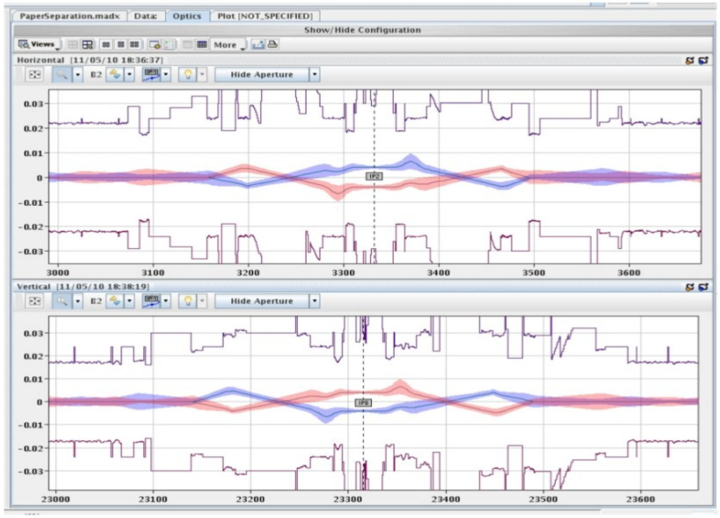
- Linear and nonlinear optics
- Matching (work in progress)
- Alignment errors, beam jitter
- Orbit correction and steering
- In the prototyping phase: space charge and CSR (with M. Dohlus I. Zagorodnov)



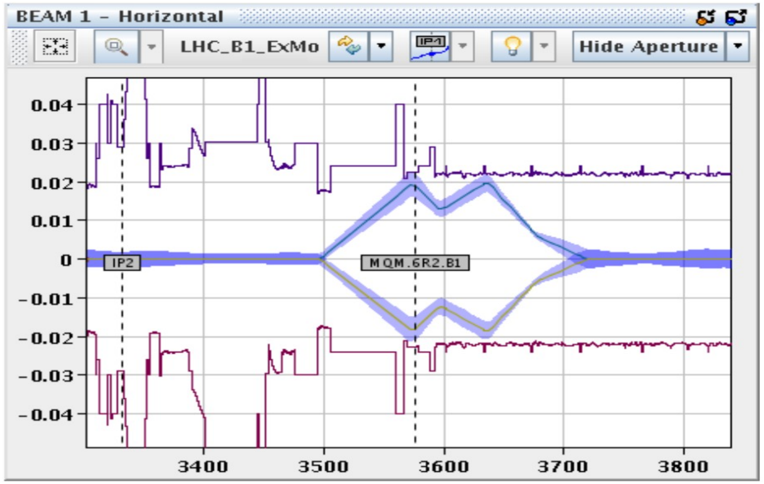
XFEL dogleg

On-line tools

- Previous experience: OM (LHC): embedding mad-x into java control system (pic below). Successful for commissioning, however software complexity and support is an issue
- Machine Interface module in xframework allows for a 'flight simulator mode' of operation (TCP-based): alignment and tuning tools could be easily transferred to control room after switching from 'virtual' to 'real' mode. Similar things have been implemented in several labs already.
- Flight simulator mode requires data exchange protocol. Optics and other features can be more easily 'embedded' in python directly
- Scripting is a major advantage for scans etc. Python used at NSLSII too.



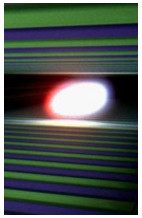
LHC OM beams at Ips

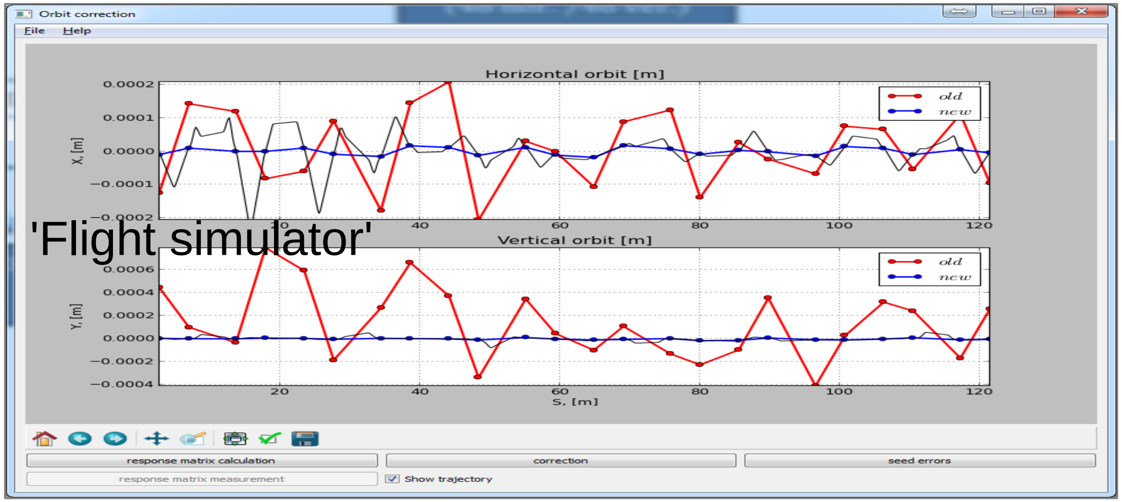


LHC OM Aperture scan

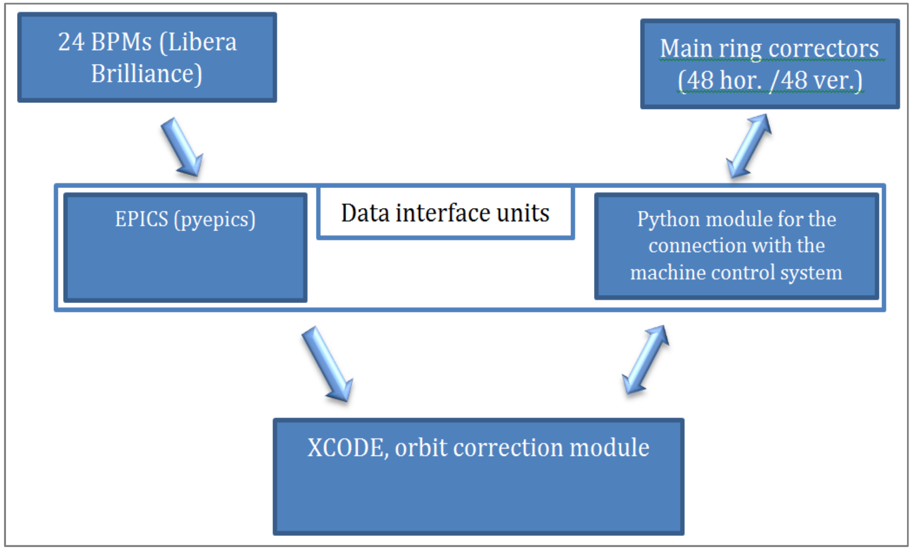
Overview of xcode

Orbit correction at sibir2





'Flight simulator'



24 BPMs (Libera Brilliance)

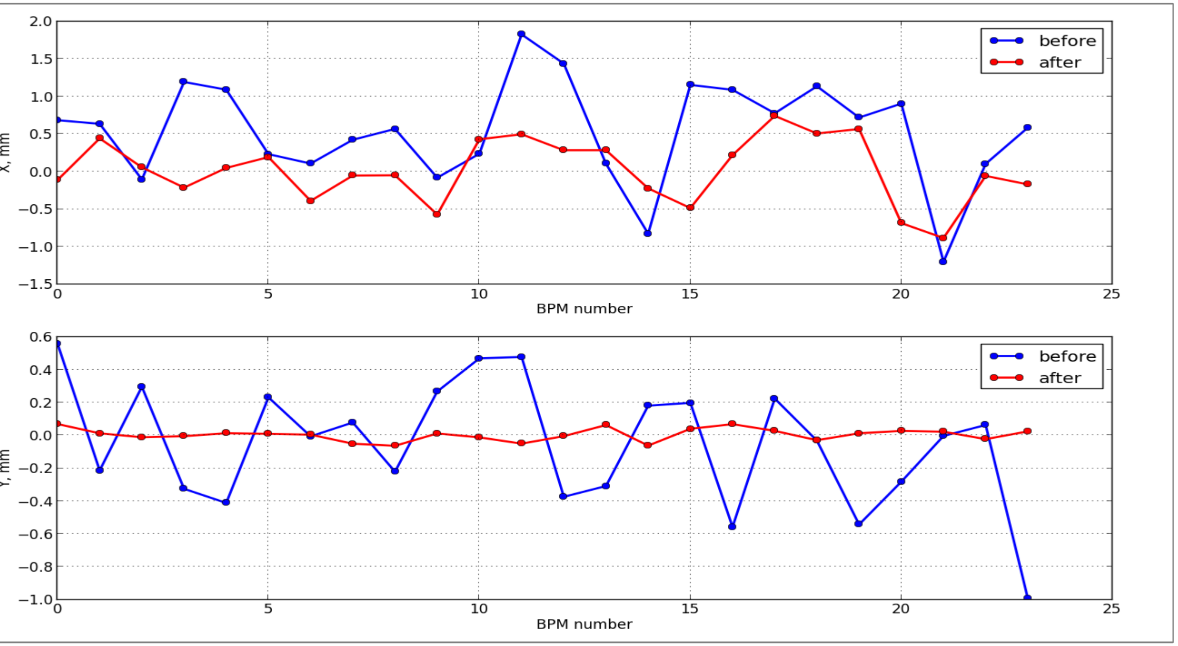
Main ring correctors (48 hor. /48 ver.)

EPICS (pyepics)

Data interface units

Python module for the connection with the machine control system

XCODE, orbit correction module



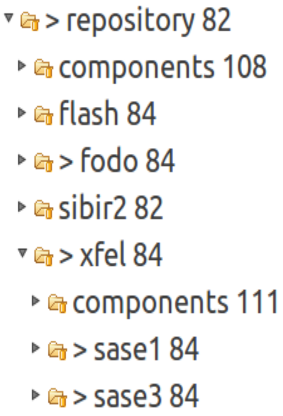
Implementation on the machine
(poor efficiency in hor. plane
since the steerers used for alignment)

	Before correction	**After correction**
σ_x, mm	**0.88**	**0.42**
σ_y, mm	**0,38**	**0.038**

Input decks

- No parsing needed
- Current input decks are derived from official MAD decks and included in repo

```
beam = Beam()
beam.E = 17.5
beam.sigma_E = 0.001
beam.I = 2.5e-10
beam.emit_x = 1.752e-11
beam.emit_y = 1.752e-11
beam.beta_x = 33.7
beam.beta_y = 23.218
beam.alpha_x = 1.219
beam.alpha_y = -0.842

und = Undulator(nperiods=73, lperiod=0.068, Kx=0.0, id = "und")
d2 = Drift (l=0.45, id = "d2")
# phase shifter
b1 = RBend (l=0.0575, angle=0.0, id = "b1")
b2 = RBend (l=0.0575, angle=-0.0, id = "b2")
psu=(b1,b2,b2,b1)
# quads
qf = Quadrupole (l=0.1, id = "qf")
qd = Quadrupole (l=0.1, id = "qd")

cell_ps = (und, d2, qf, d2, und, d2, qd, d2)
sase3 = (und, d2, qd, d2) + 11*cell_ps
```

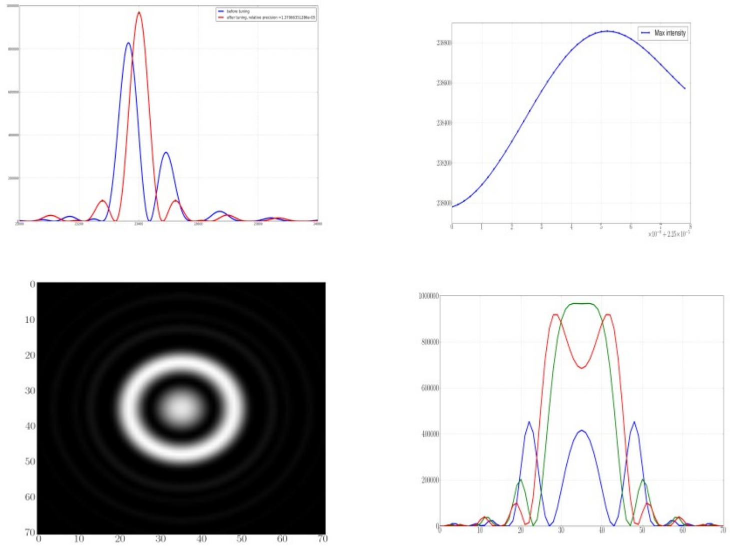


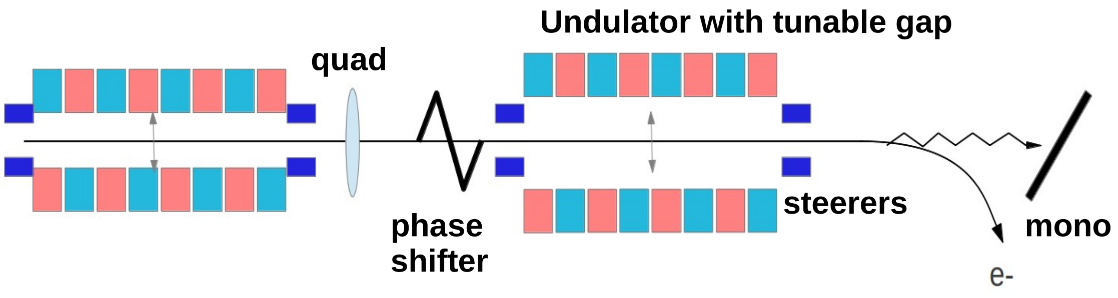
- > repository 82
  - components 108
  - flash 84
  - > fodo 84
  - sibir2 82
  - > xfel 84
    - components 111
    - > sase1 84
    - > sase3 84

SR/PBBA

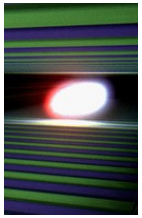
- Main motivation of SR is for diagnostics
- Tuning undulator K and phase shifter based on SR properties
- Any study cases should be easily transferrable to the control room
- Prototype in place for integrating into controls (Karabo, doocs)

SR properties for various phase shifter strengths





Embedding python is simple



- Twiss calculation

```
exec( open("../../repository/flash/flash.inp" ))
tw0 = Twiss(beam)
lat = MagneticLattice(flash_sase, beam.E)
tws=twiss(lat, tw0)
```

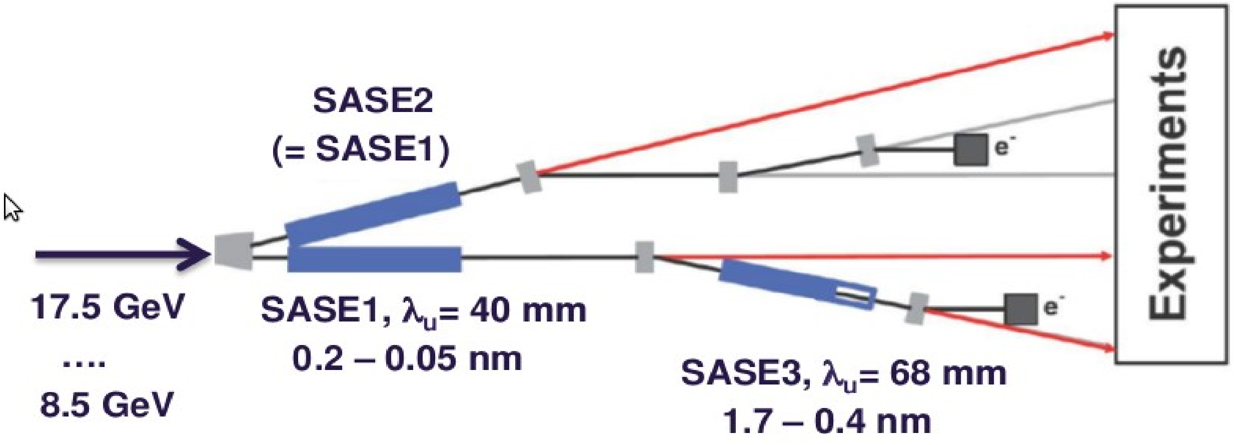
- Running a SR calculation and saving into hdf5

```
traj, int1 = srw.calculateSR_py(lat, beam, screen, runParameters)

dump = Dump()
dump.readme = 'test 1_1'
dump.index['beam'] = beam
dump.index['screen'] = screen
dump.index['intensity'] = int1
dump.index['trajectory'] = traj

xio = XIO('data/int_test_1_1.h5')
dump.dump(xio)
```

II/IV
Radiation properties at XFEL

European XFEL

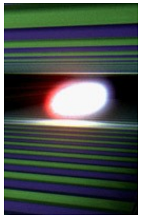
- 17.5 GeV superconducting accelerator
- 10 Hz, 600mus trains with 220ns bunch spacing
- Result of more than a decade long RnD with installation currently underway and first lasing expected 2016



Radiation parameter calculation

- First stage: important basic feasibility and proof of principles (flash/ttf). Very simplified modelling sufficient
- Now following software needs could be identified:
  - Various alignment and tuning tools
  - Upgrade scenarios
  - More detailed fel simulations taking increasing understanding of the machine Into account
  - Presentation for users required

Radiation parameter calculation

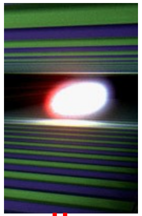


- FEL theory exists but can describe radiation realistic 3d distributions only qualitatively
- Steady state (without longitudinal dimension) and 1D (without 'diffraction effects')

Computationally simpler and often helpful for qualitative analysis

- Main complications are
  - Non-gaussian bunches due to CSR and other effects in linac
  - Segmented undulators with e beam focusing
  - Gap tapering and other manipulations

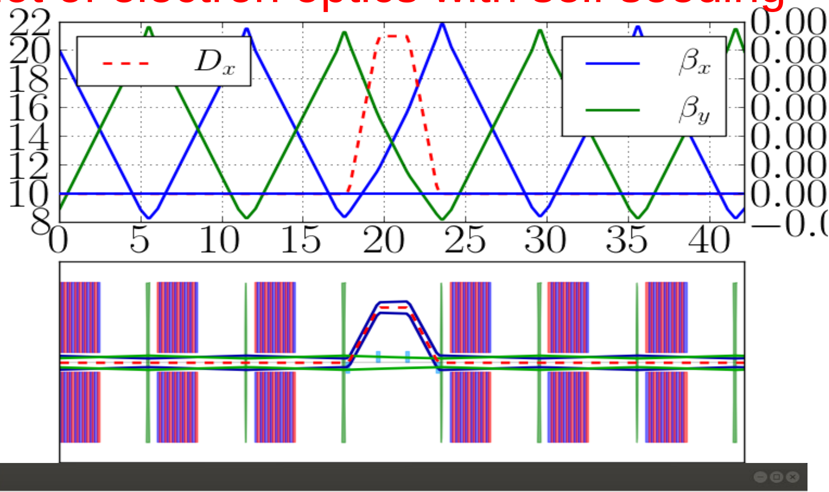
$$\lambda_r = \frac{l_w}{2\gamma^2}\left(1 + \frac{K^2}{2}\right) \qquad \rho = \frac{1}{\gamma}\left(\left(\frac{K A_{JJ} l_w}{8\pi\sigma_b}\right)^2 \frac{I}{I_A}\right)^{\frac{1}{3}} \qquad L_G = l_w/(4\pi\sqrt{3}\rho)$$

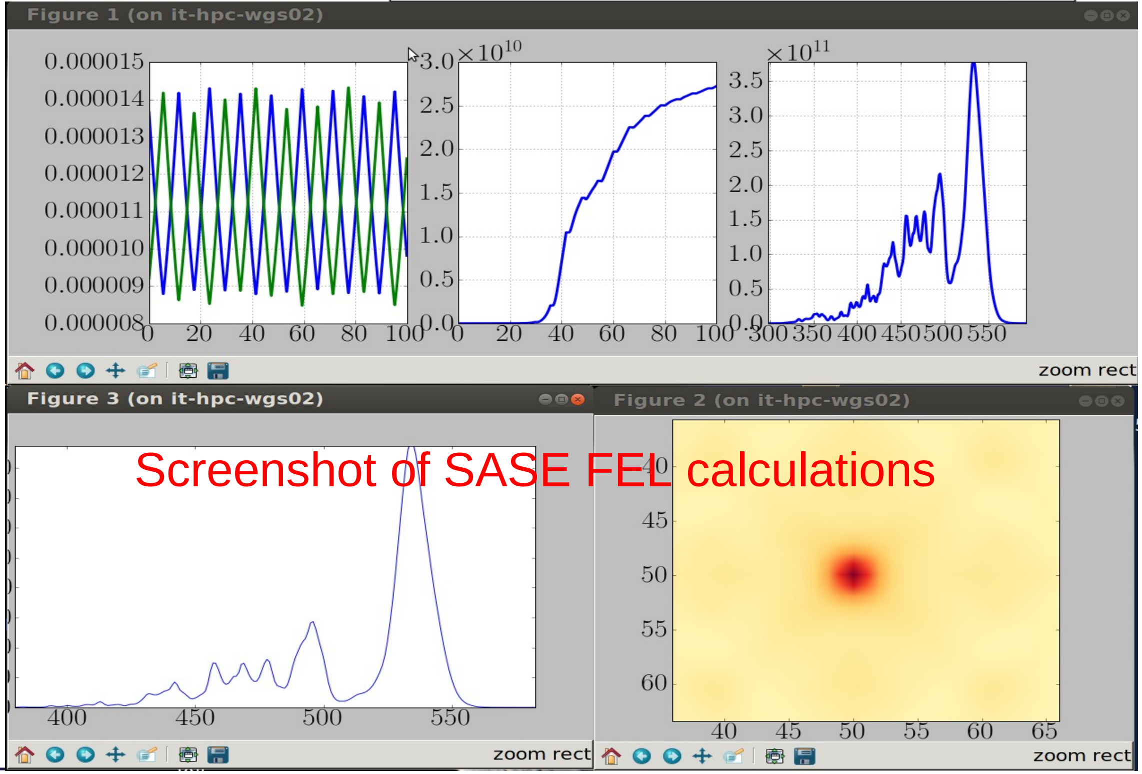


FEL simulations in xcode/genesis

- Based on same model asSR/FEL/electron beam dynamics
- Feature of FEL calculations:
    - Python interface to genesis
    - Optics model from standard repository
    - Rematching optics
    - Parameter scans
    - Postprocessing/plotting
    - Interface to 'wavefront propagation'
    - On-line use possible (commissioning). Few minutes response time (cluster) for checking a particular scenario (electron beam parameters, wavelength, undulator configuration)

Screenshot of electron optics with self seeding





Screenshot of SASE FEL calculations

Cross-checking with previously made FAST calculations

Saturation parameters are similar to 'official parameters', but

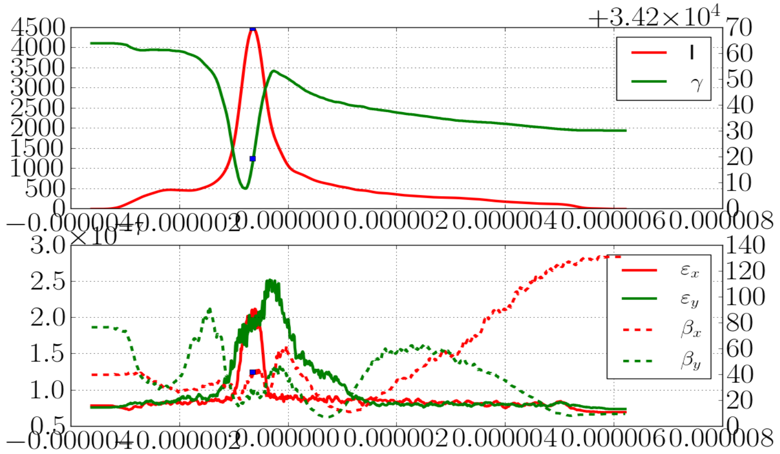
1) electron beam parameters give some range of variation

2) especially short pulses can be non-gaussian in time/frequency/space which leaves space for interpretation of width

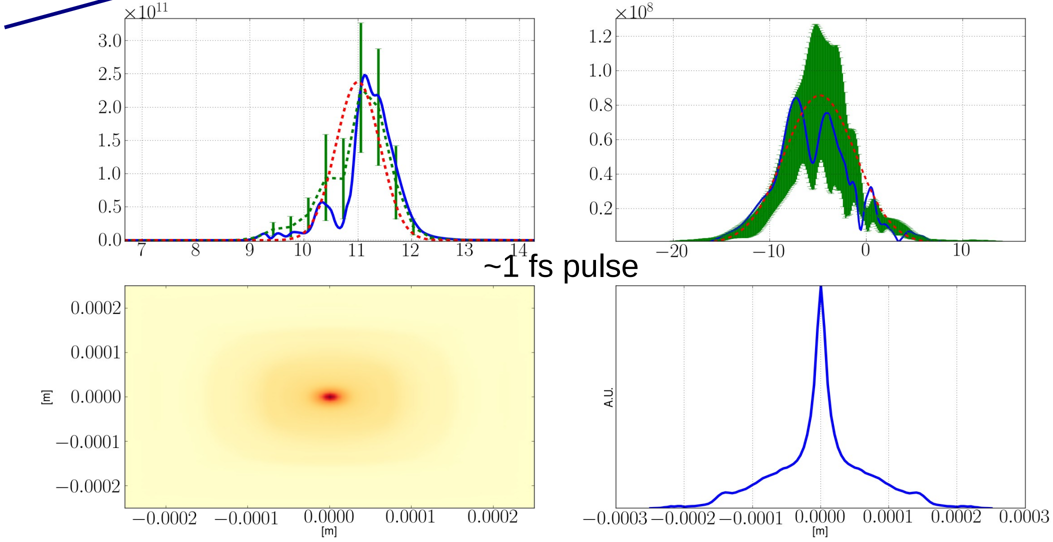
WP	$\epsilon_{x,y}[10^{-6}]$	$\sigma_E[MeV]$	L_{sat}	$N_\gamma \times 10^{12}$	$\frac{\Delta\omega}{\omega}$ [%]	τ_γ[fs]
0.02nC 1.6 fs	0.32/0.32	2	42.0	2.6	0.4	0.97 - 1.58
	0.2 / 0.18	2	36.0	2.46	0.36	1.22 - 1.35
	0.32 / 0.32	10	48.0	1.44	0.32	1.26
0.1nC 8 fs	0.39/0.39	2	48.0	15	0.22 - 0.92	12.7
	0.32/0.27	2	42.0	14.6	0.44 - 0.92	10.1
	0.39/0.39	10	54	12	0.4 - 0.84	9.7
0.25nC 20 fs	0.6/0.6	2	48.0	23	0.3 - 0.7	25.8
	0.4/0.36	2	42.0	23	0.2 - 0.8	20.6
	0.6/0.6	10	54.0	18	0.04 - 0.5	14-17
0.5nC 40 fs	0.7/0.7	2	48.0	30	0.2-0.4	33-38
	0.45/0.42	2	42	31	0.32-0.6	33
	0.7/0.7	10	—			
1nC 80 fs	0.97/0.97	2	54	80	0.2 - 0.4	69 - 94
	0.8/0.84	2	48	40	0.34 - 0.4	64-69
	0.97/0.97	10	66	50	0.2 - 0.35	60 - 75

Energy spread depends
On sase1 mode

Accelerator simulations
c/o Feng/Zagorodnov



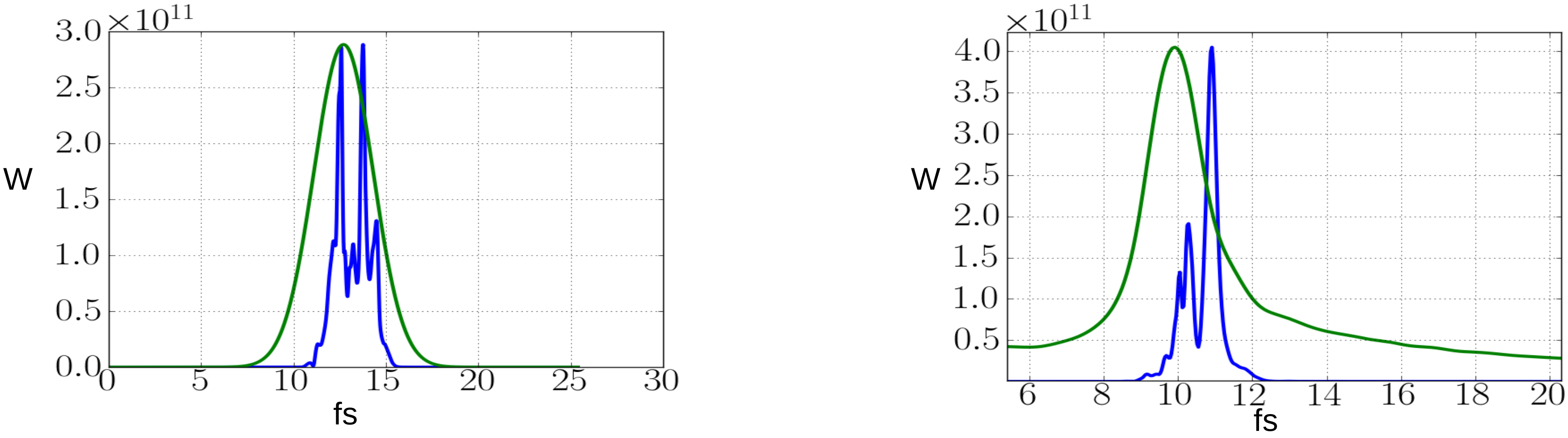
750eV



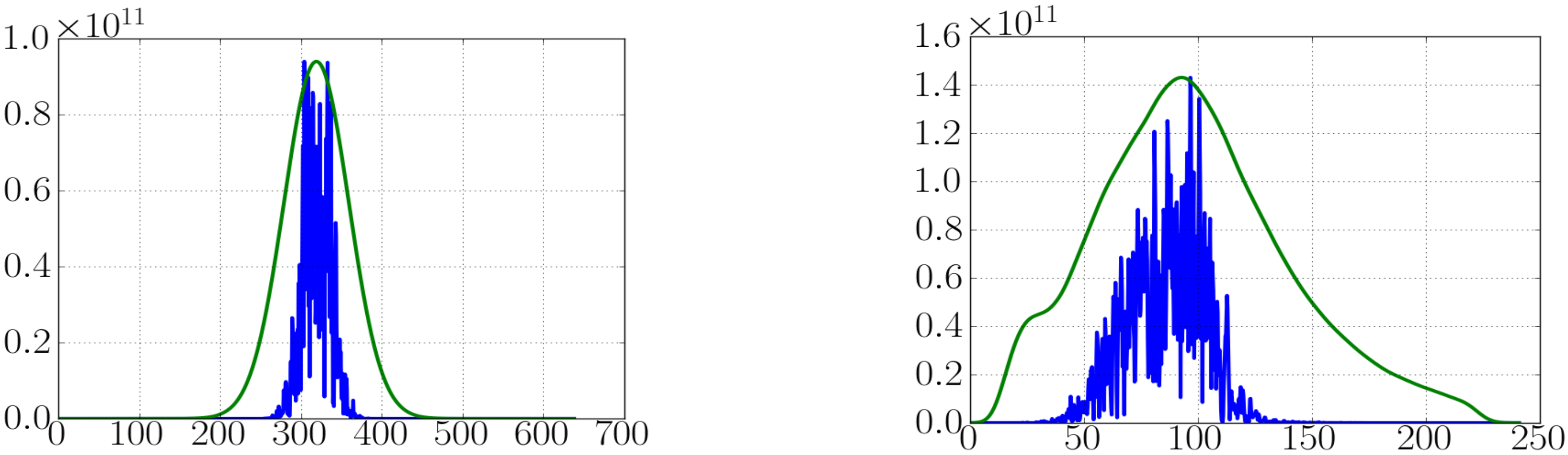
~1 fs pulse

Example: parameters for SASE3 (soft x-ray)

1500eV, ~1fs. Roughly next undulator exit after saturation



1500eV, ~40fs

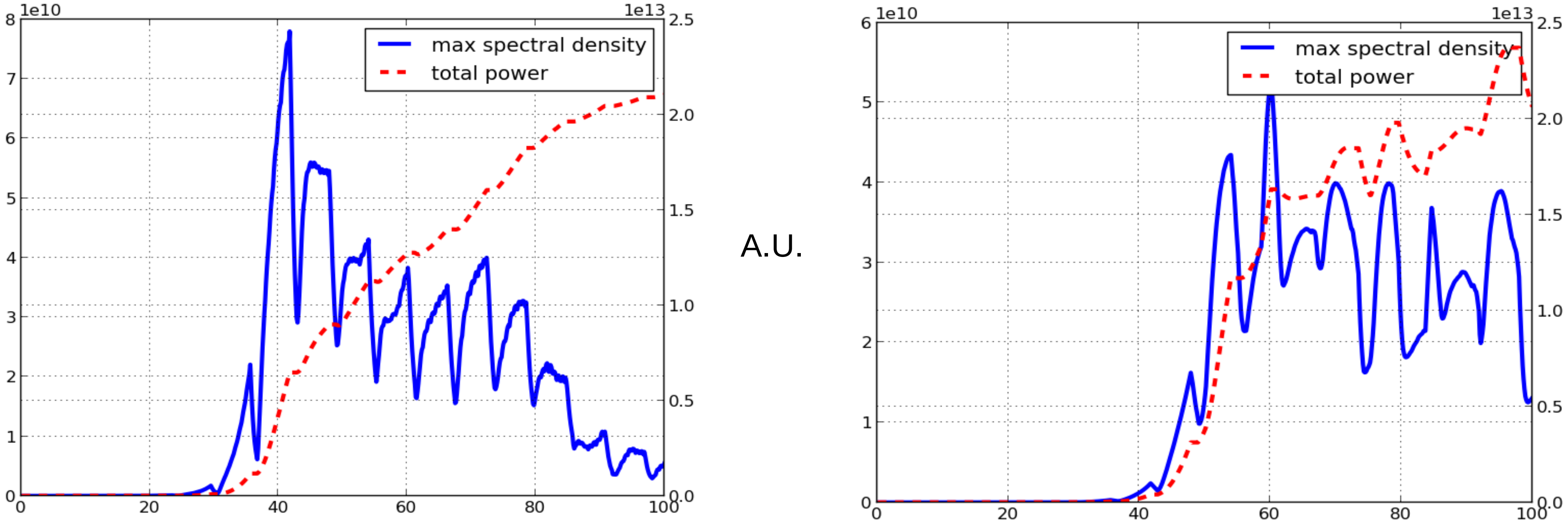


Example: parameters for SASE3

Saturation parameters need not correspond to the working point

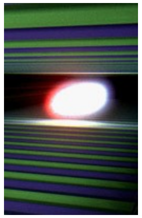
1) self-seeding and tapering (work in progress to incude in the framework)

2) for sase, in operation tuning saturation point exactly to undulator exit is probably not possible. Missing that by few meters can result in x2 in power.



750eV, different pulse durations

Post-saturation tapering

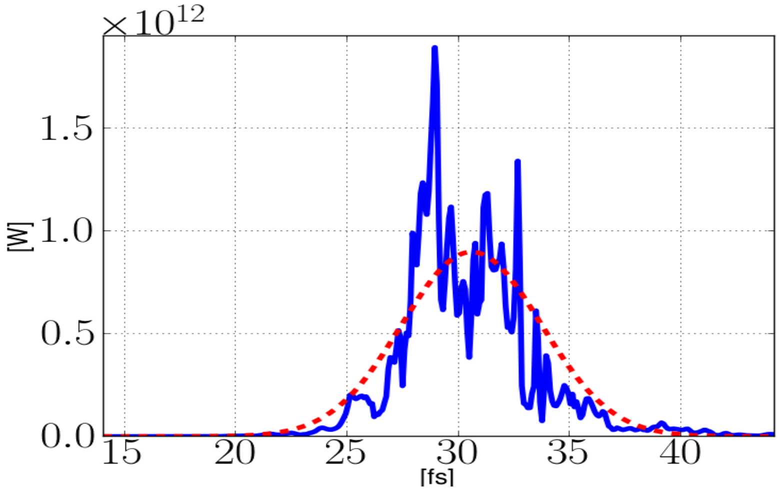


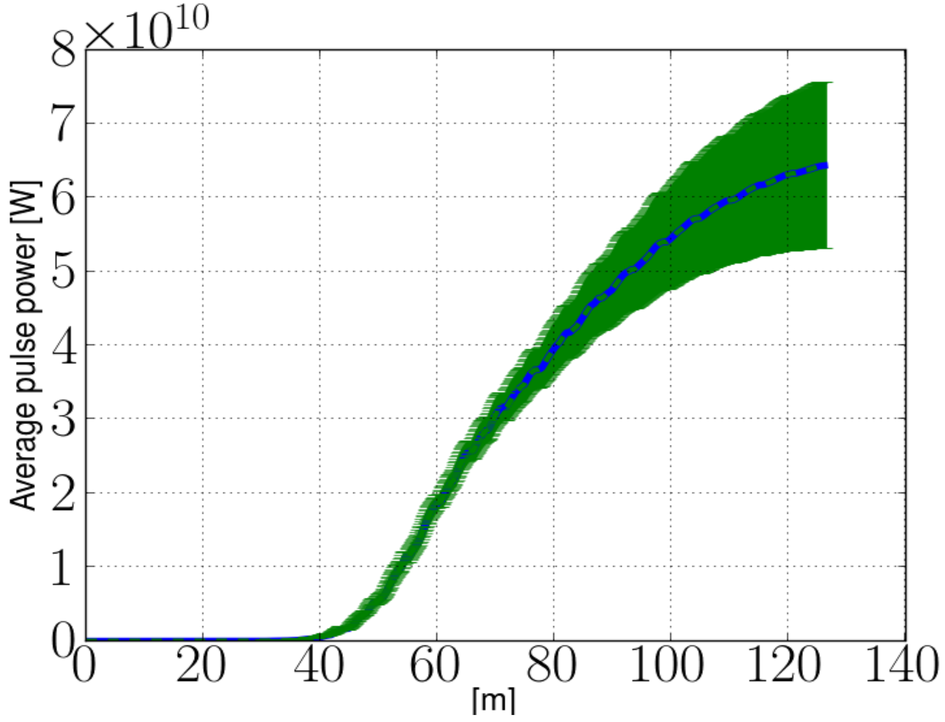
By tapering the undulator gap one in the 'nonlinear regime'

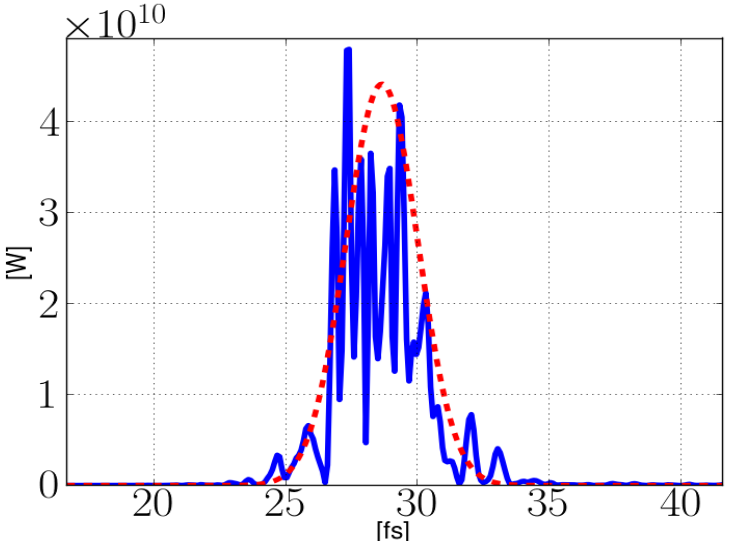
The power growth is linear

Up to tenfold increase in total/peak power

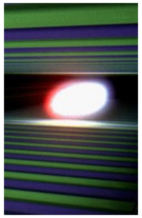
And spectral density



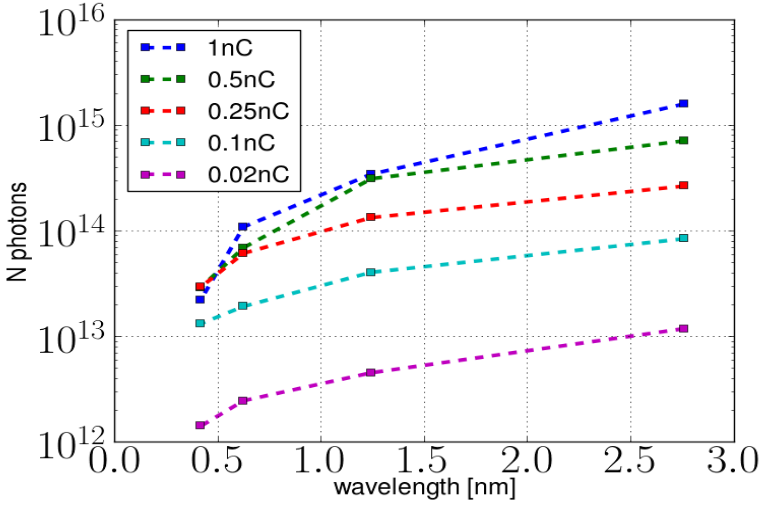


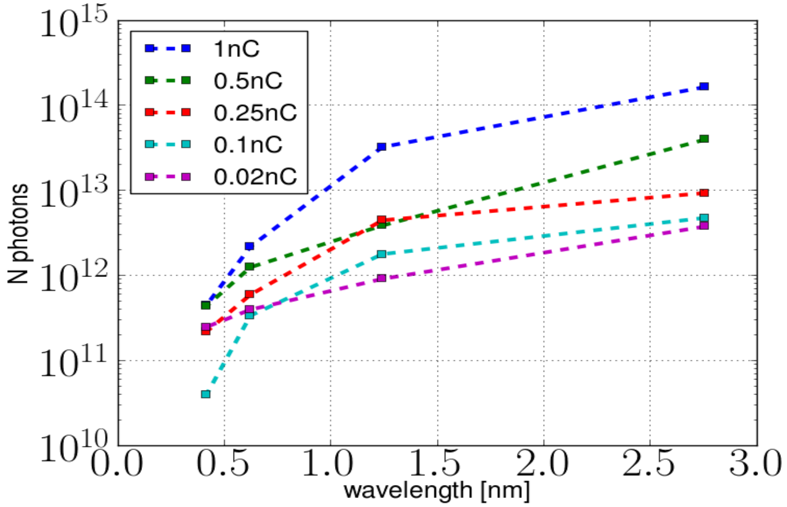


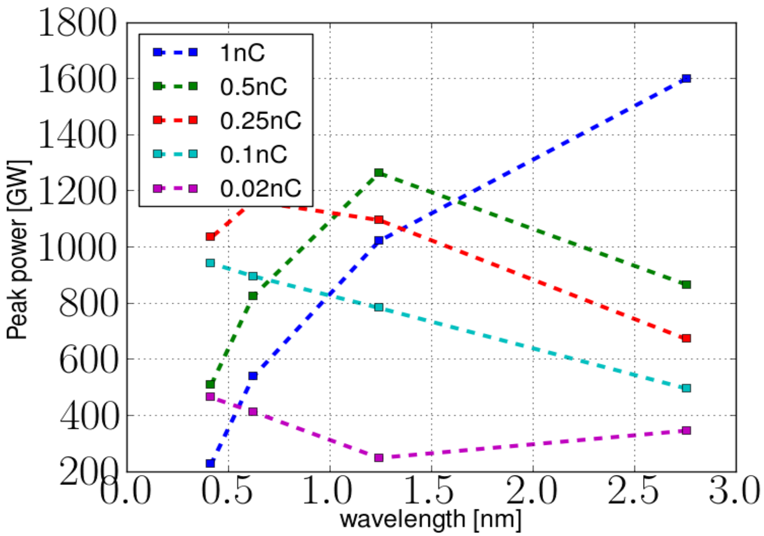
Post-saturation tapering

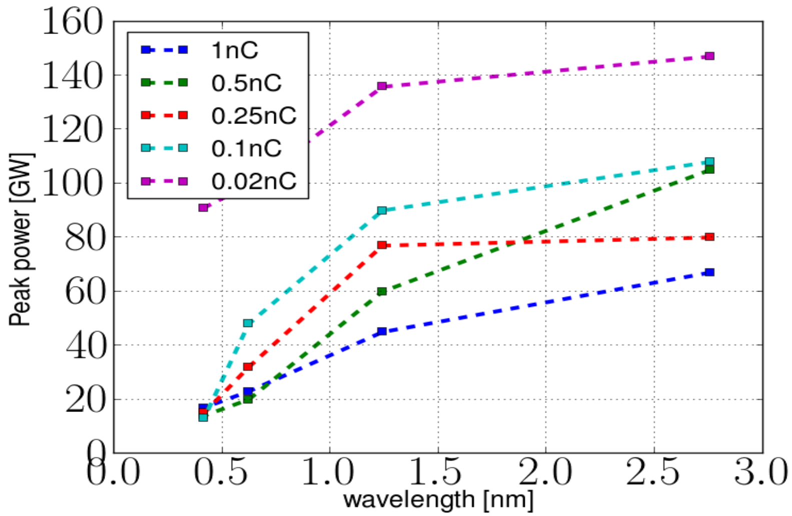


Challenge: source characterization for all working points

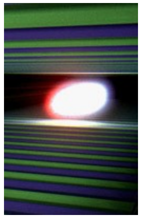




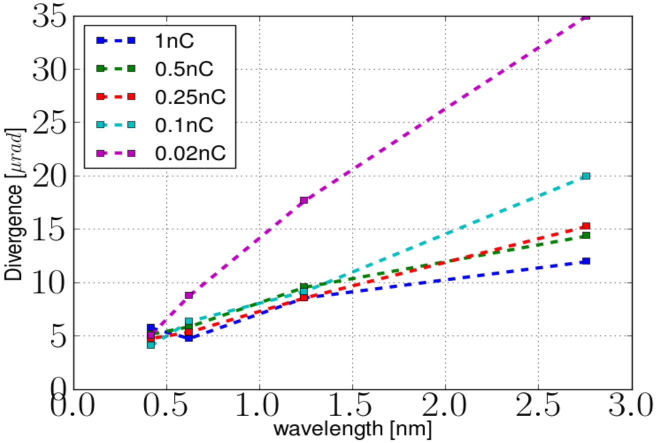


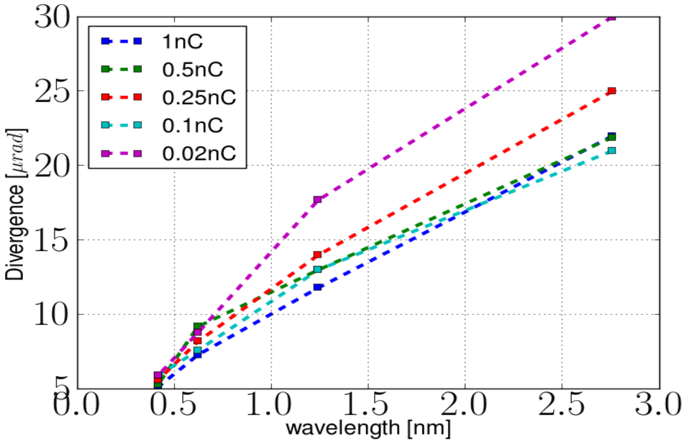


Post-saturation tapering

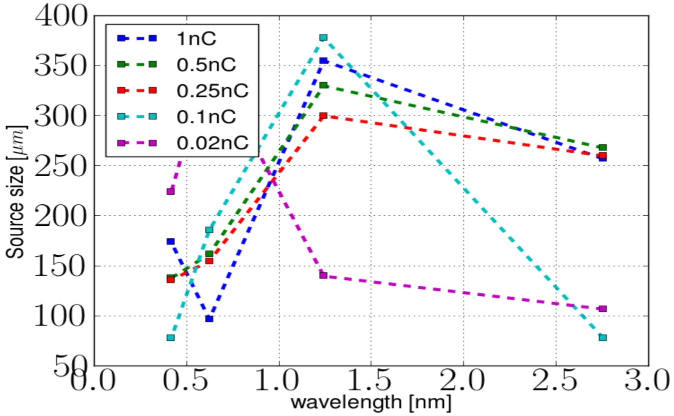


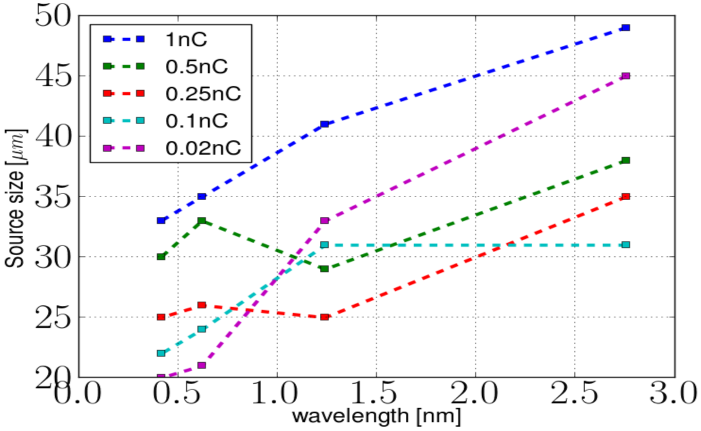
Divergence (important for x-ray optics design) stays the same as in saturation





Source size (important for tight focus) is less understandable and needs further study. Figure below shows photon beam size at a certain distance from undulator exit





Self-seeding techniques and their importance for XFELs

SASE pulses, baseline mode of operation: poor longitudinal coherence

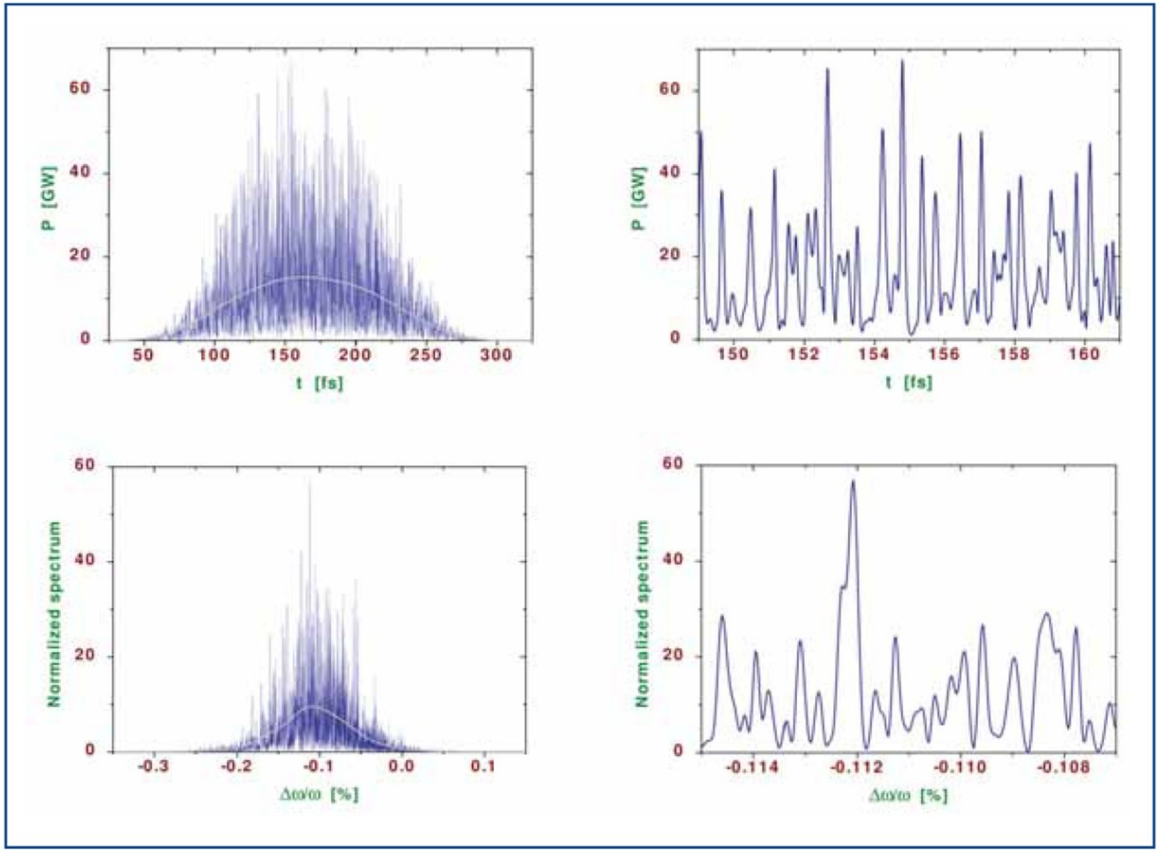


Figure 5.2.4 *Temporal (top) and spectral (bottom) structure for 12.4 keV XFEL radiation from SASE 1. Smooth lines indicate averaged profiles. Right side plots show enlarged view of the left plots. The magnetic undulator length is 130 m.*

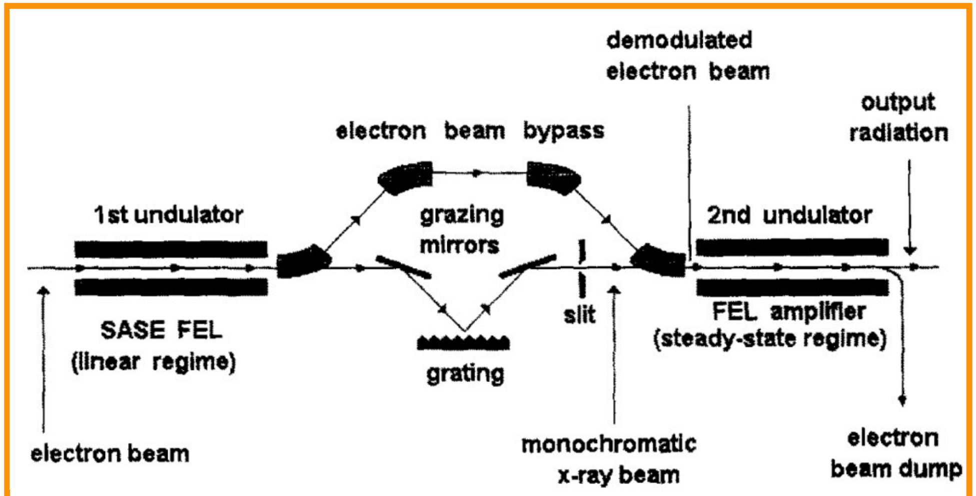
Source: The European XFEL TDR – DESY 2006-097 (2006)

$$\frac{\Delta\omega}{\omega} \sim 2\rho \sim 10^{-3}$$

$$\left(\frac{\Delta\omega}{\omega}\right)_{spike} \sim \frac{1}{\sigma_T \omega} \sim 10^{-5}$$

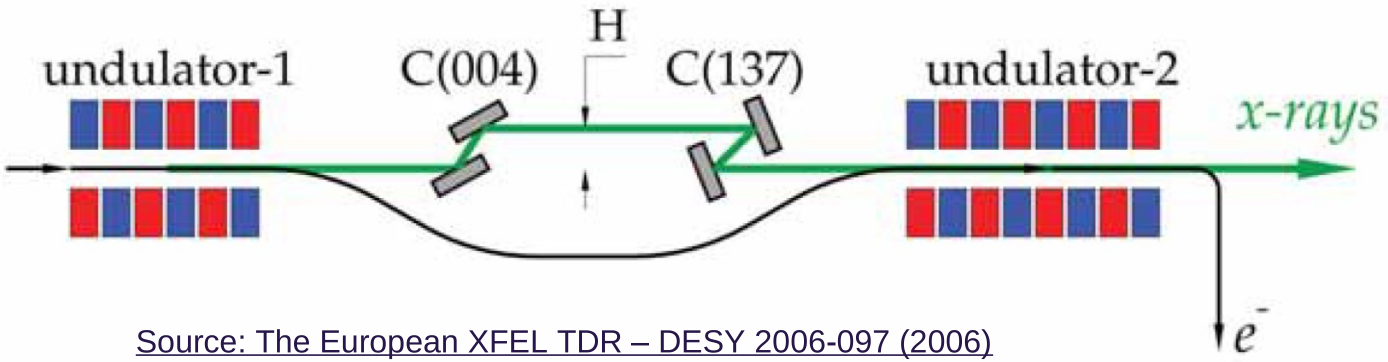
- Hundreds of longitudinal modes
- A lot of room for improvement
- Self-seeding schemes answer the call for increasing longitudinal coherence

Single-bunch self-seeding with a four-crystal monochromator



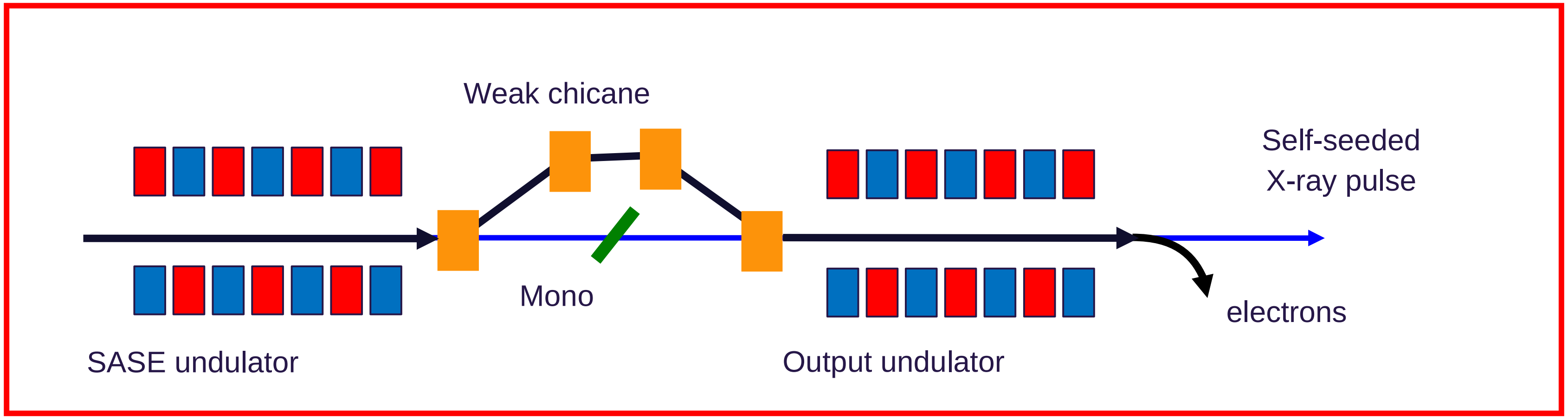
Source: J. Feldhaus et al., Optics Comm. 140 (1997)

- Method historically introduced for soft x-rays in: J. Feldhaus et al., Optics Comm. 140, 341 (1997)
  - Linearly amplified SASE is filtered through a grating monochromator
  - Electron beam bypass washes-out beam microbunch makes up for x-ray path delay by grating and allows for grating installation
  - Demodulated beam is seeded in the output undulator
- Grating monochromator substituted by crystal monochromator for applications to hard-x rays: [E. Saldin, E. Schneidmiller, Yu. Shvyd'ko and M. Yurkov, NIM A 475 357 (2001)]
- Extra x-rays path due to mono ~1cm. Long electron bypass (tens of meters) needed



Source: The European XFEL TDR – DESY 2006-097 (2006)

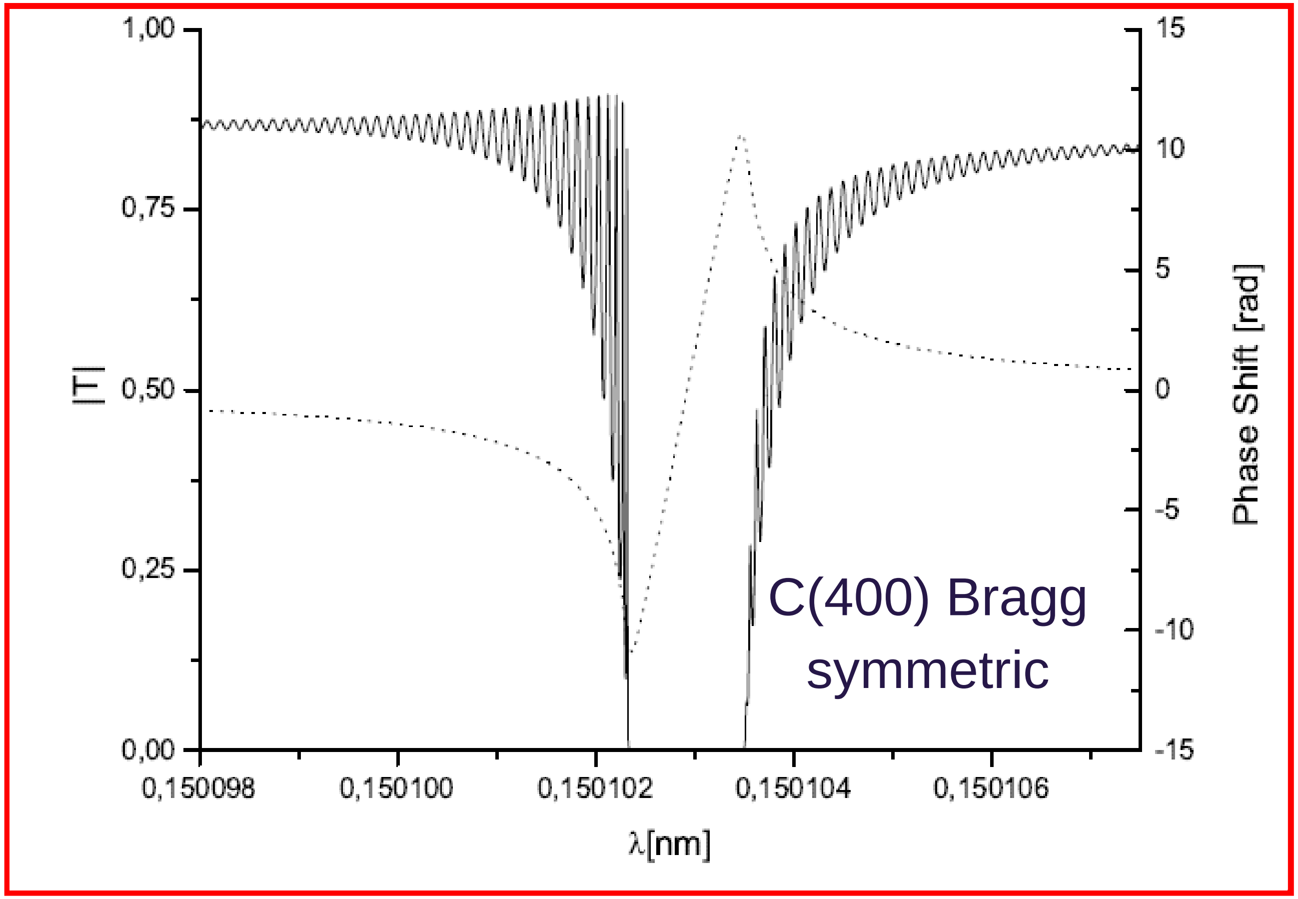
Working principle (I)

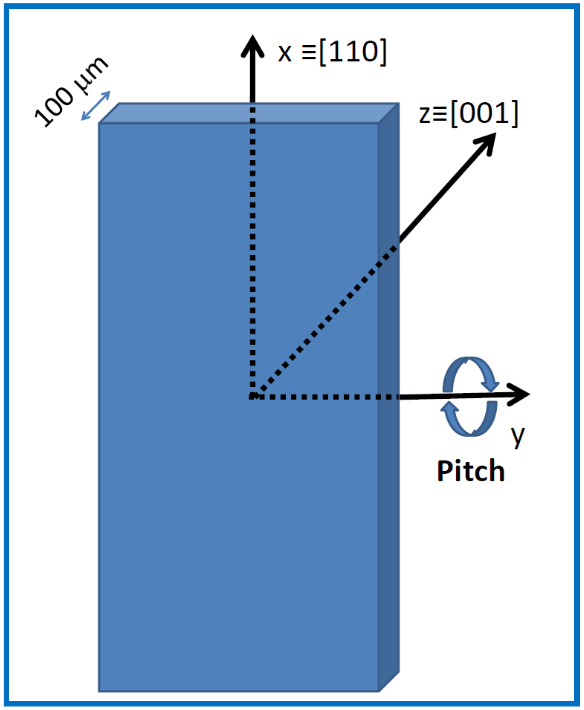


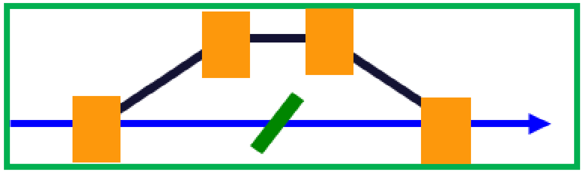
- First part: usual SASE → linear regime pulse
- Weak chicane needed for:
    - Creating a small offset (a few mm) to insert the monochromator
    - Washing out the electron beam microbunching
    - Acting as a tunable delay line
- The photon pulse from SASE goes through the monochromator
- Photon and electron pulses are recombined

Proposed in: . Geloni, G., Kocharyan V., and Saldin, E., "A novel Self-seeding scheme for hard X-ray FELs", Journal of Modern Optics, vol. 58, issue 16, pp. 1391-1403, DOI:10.1080/09500340.2011.586473 (2011)

Working principle (II)



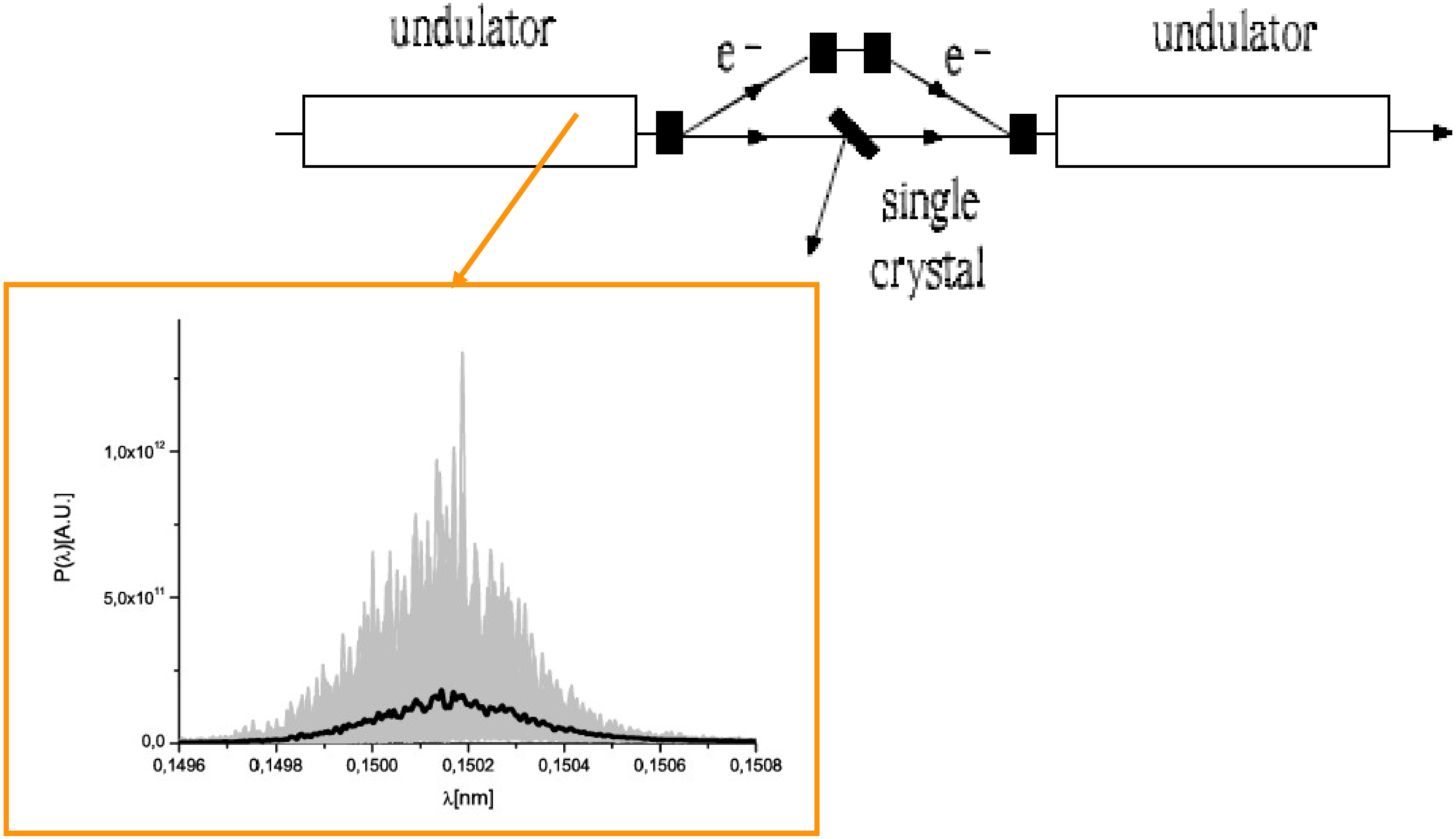




The monochromator hardware is constituted by a single crystal. The forward diffracted beam is considered. In the space-frequency domain, the crystal acts as a multiplicative filter (modulus and phase). Characterization of the filter needed.

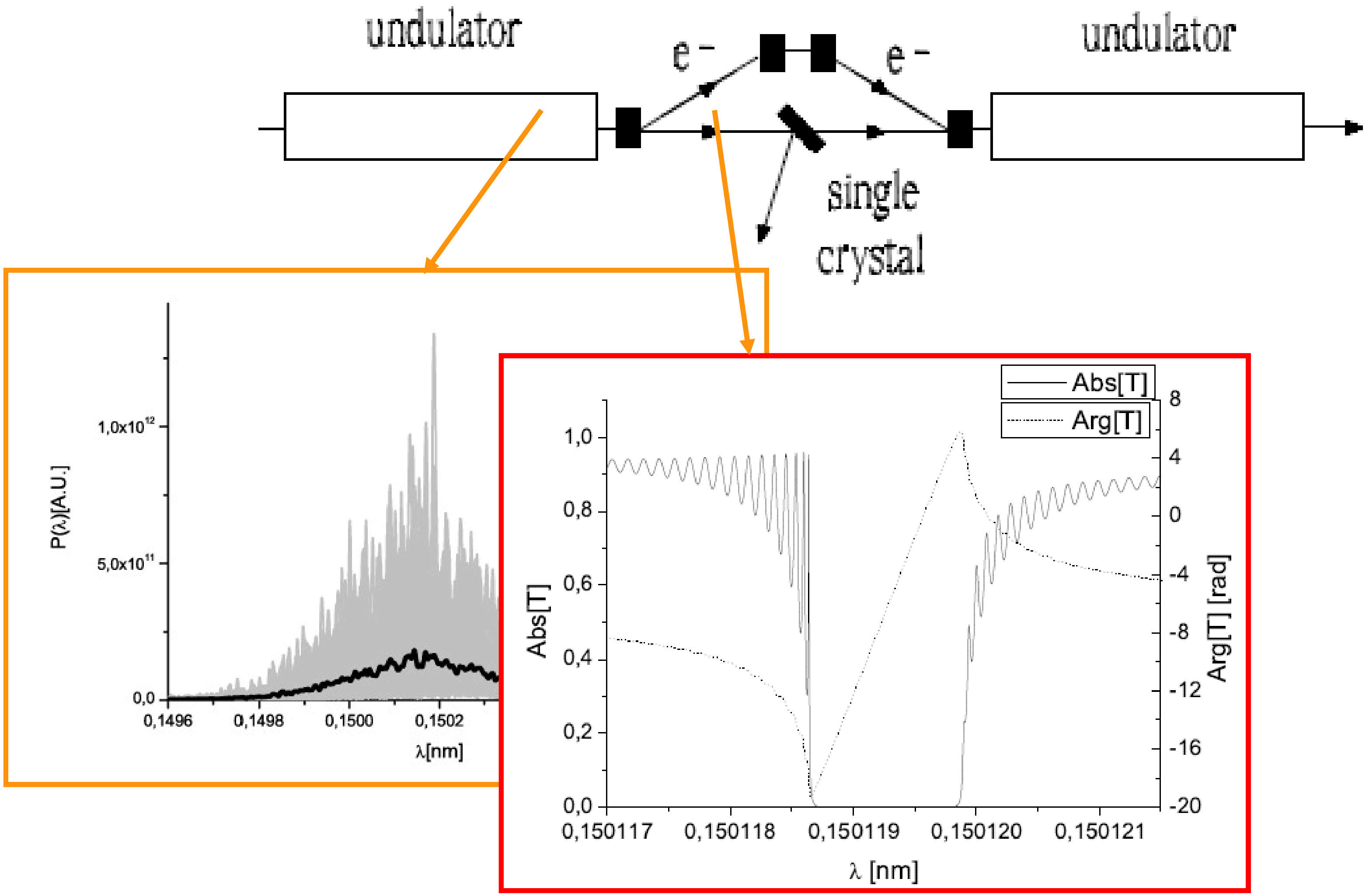
Working principle (III)

The single-crystal monochromator principle: frequency domain



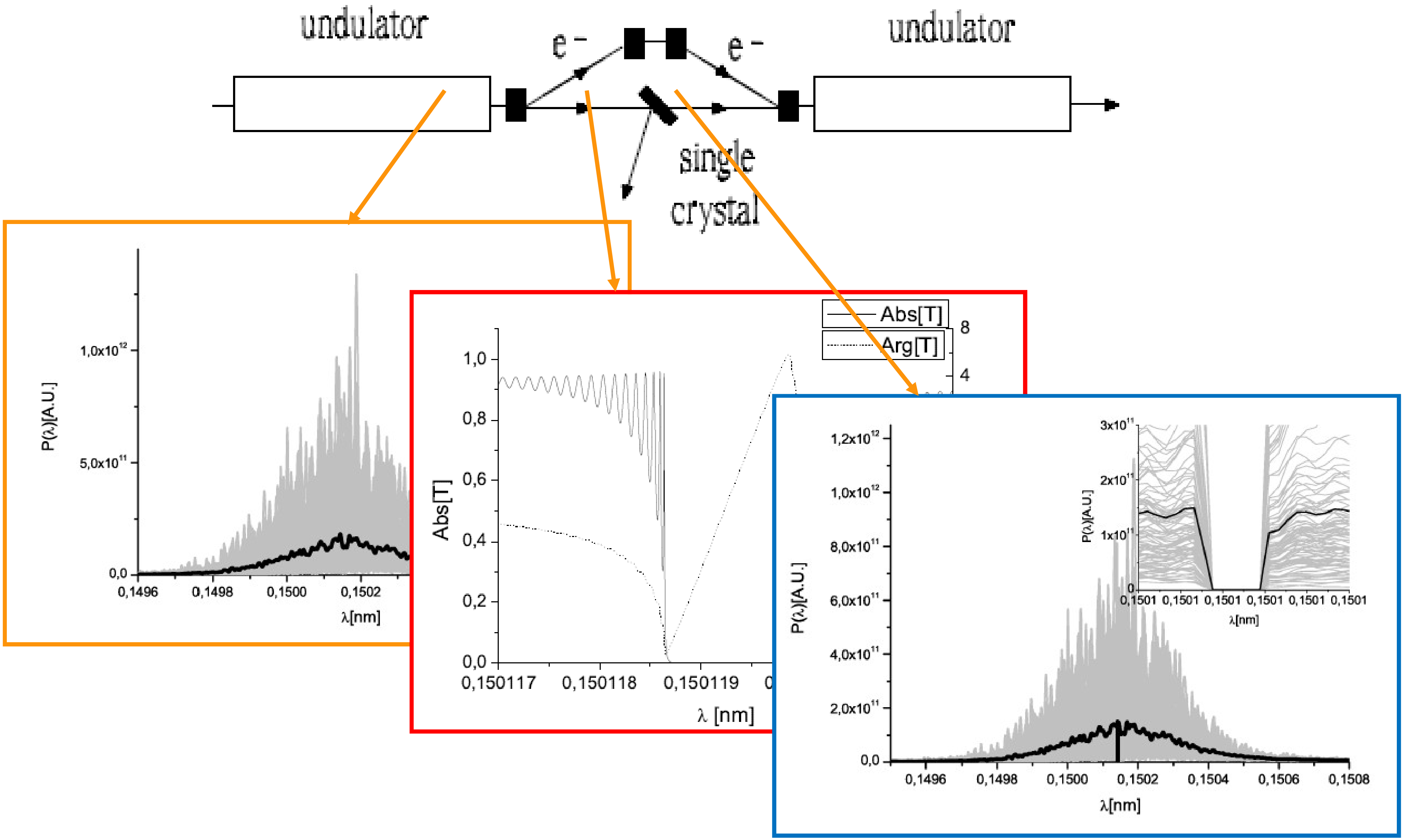
Working principle (III)

The single-crystal monochromator principle: frequency domain



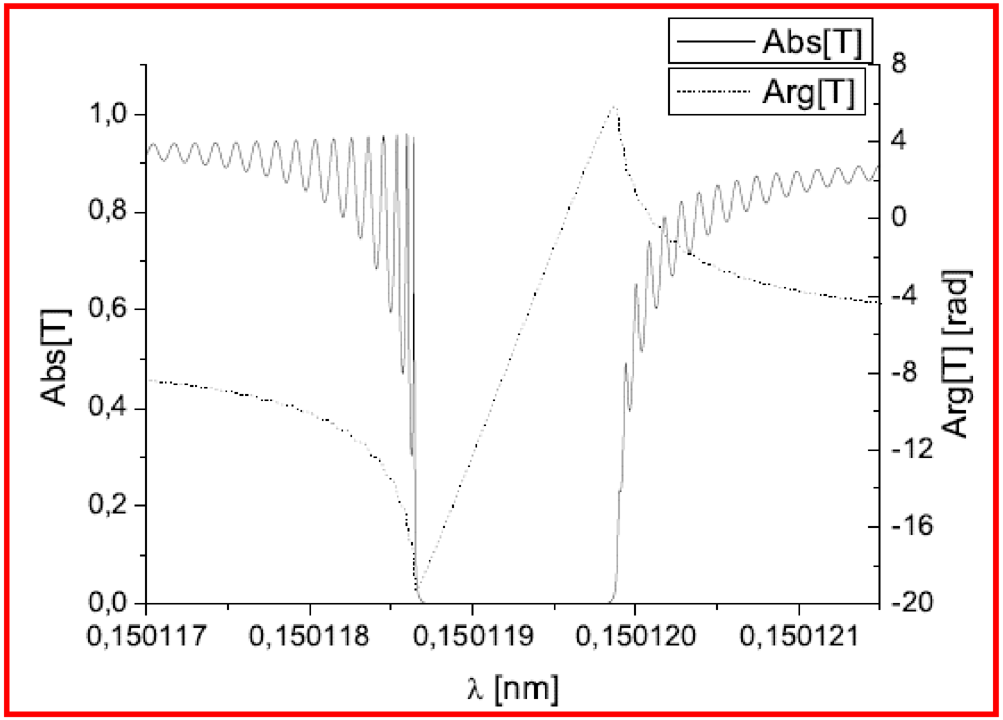
Working principle (III)

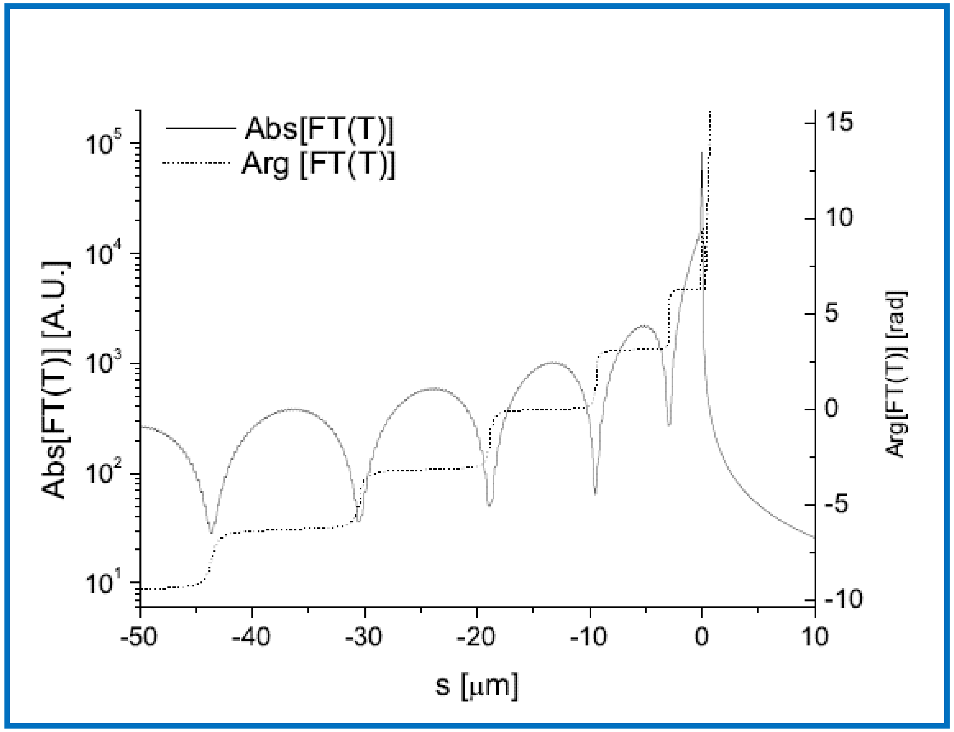
The single-crystal monochromator principle: frequency domain



Working principle (IV)

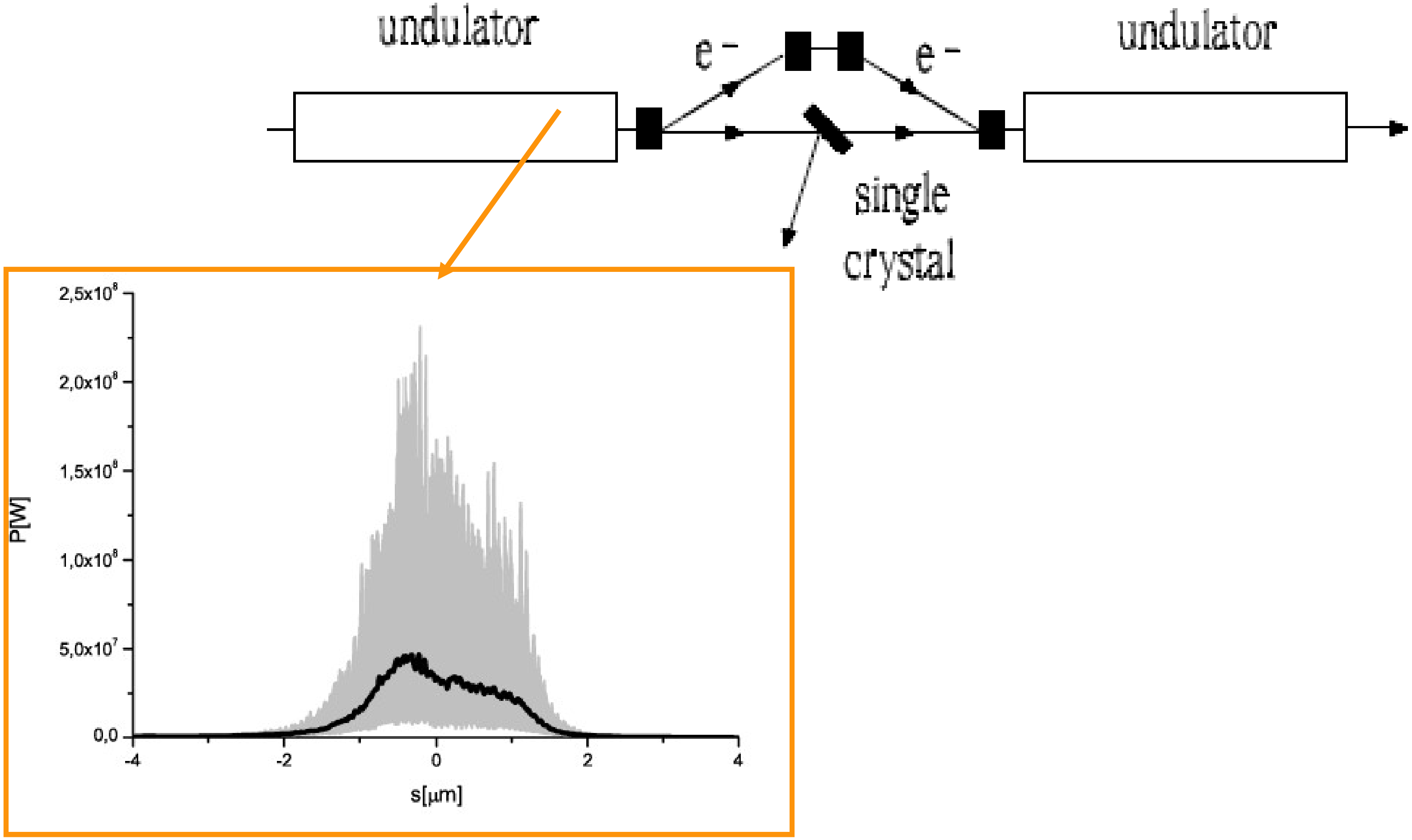
The single-crystal monochromator principle: what happens in the time domain?





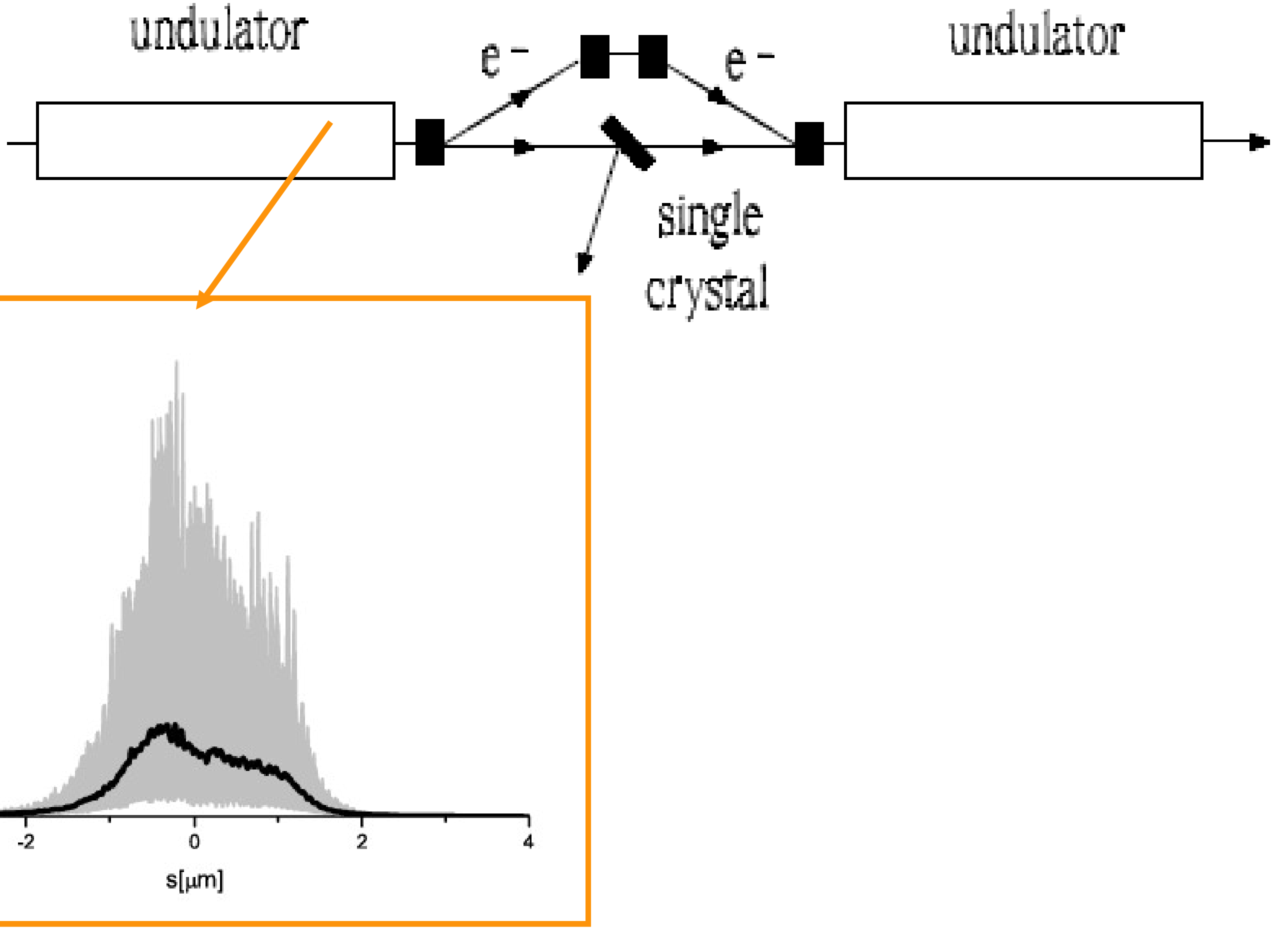
Working principle (V)

The single-crystal monochromator principle: time domain



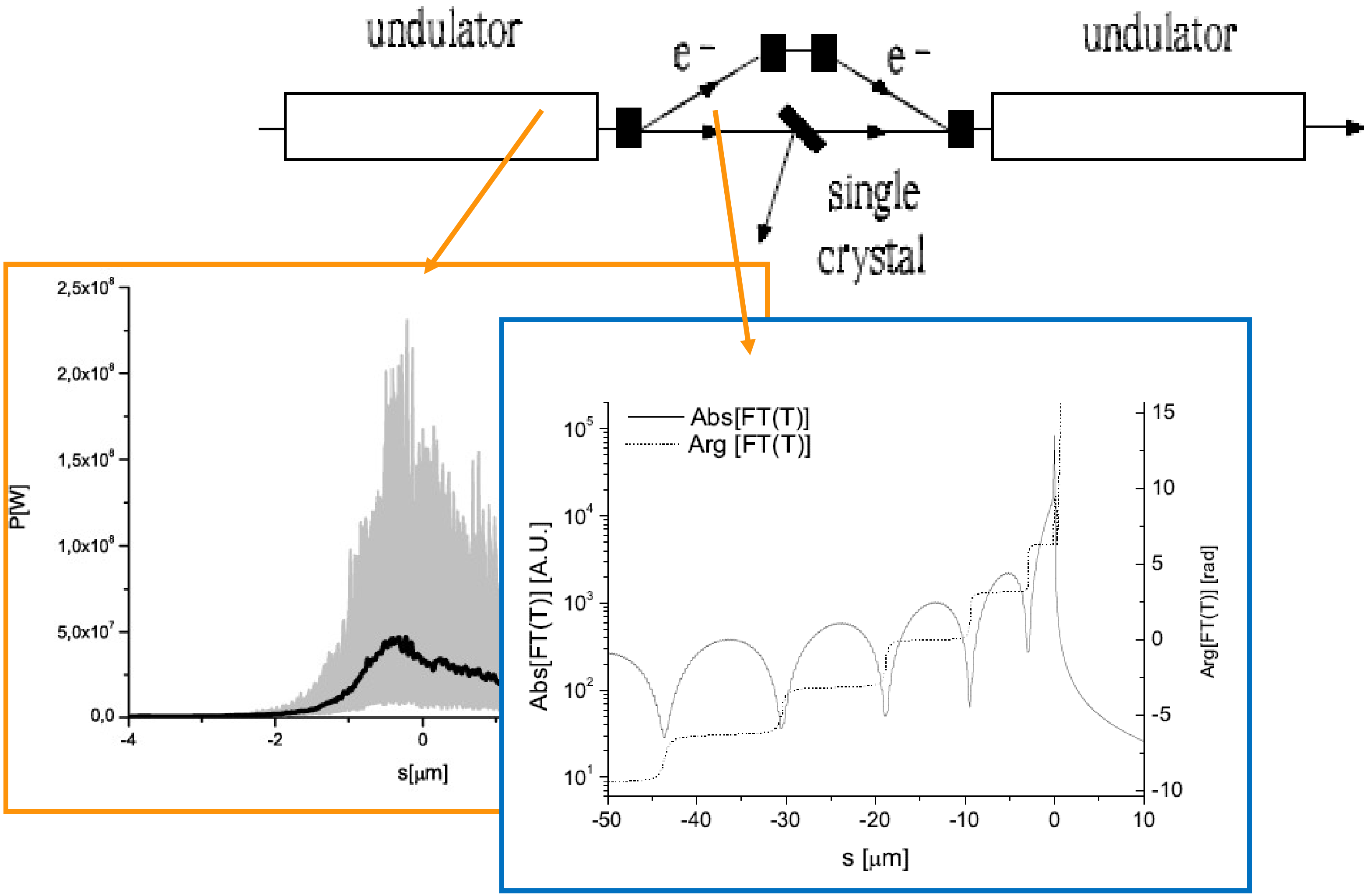
Working principle (V)

The single-crystal monochromator principle: time domain



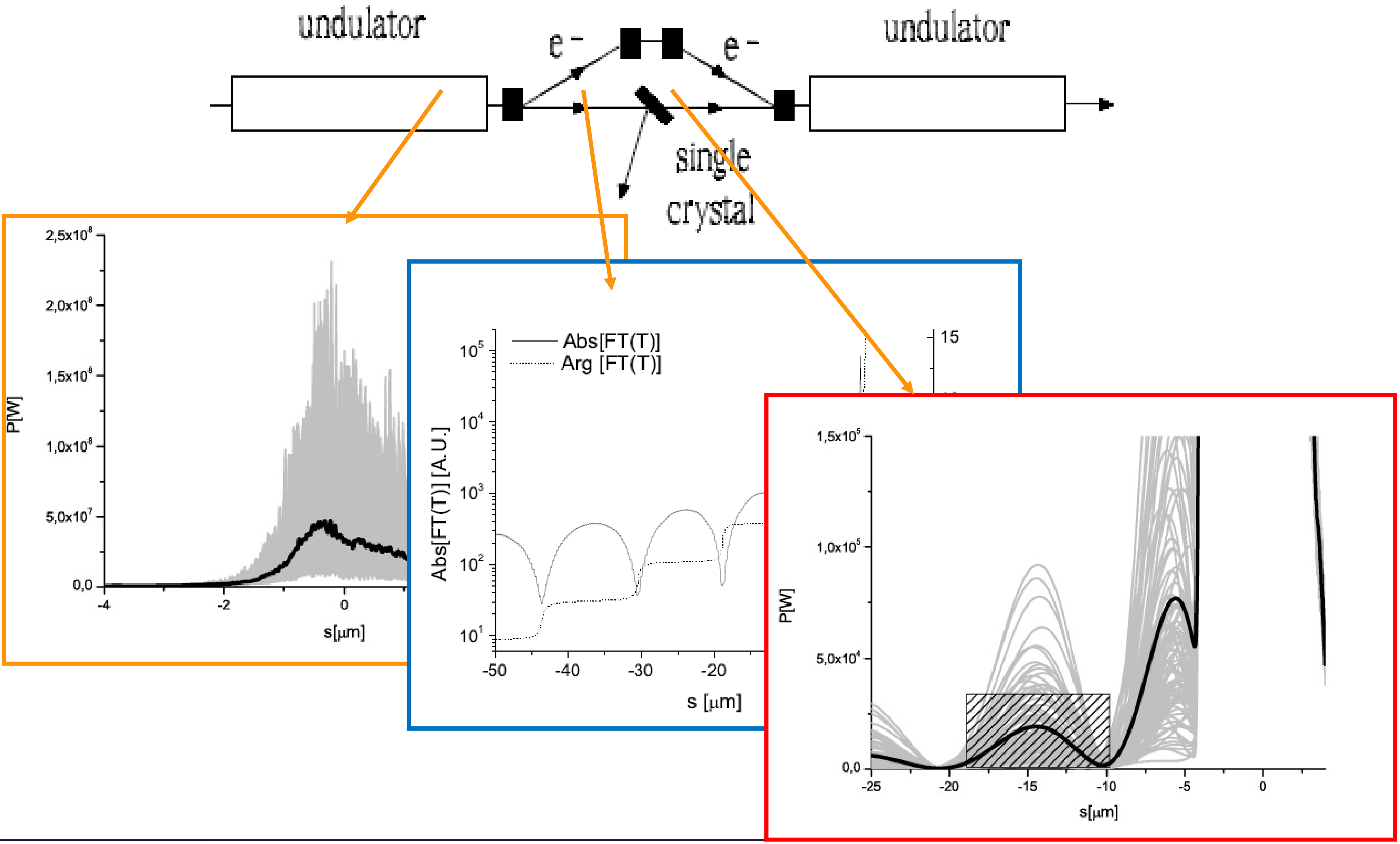
Working principle (V)

The single-crystal monochromator principle: time domain



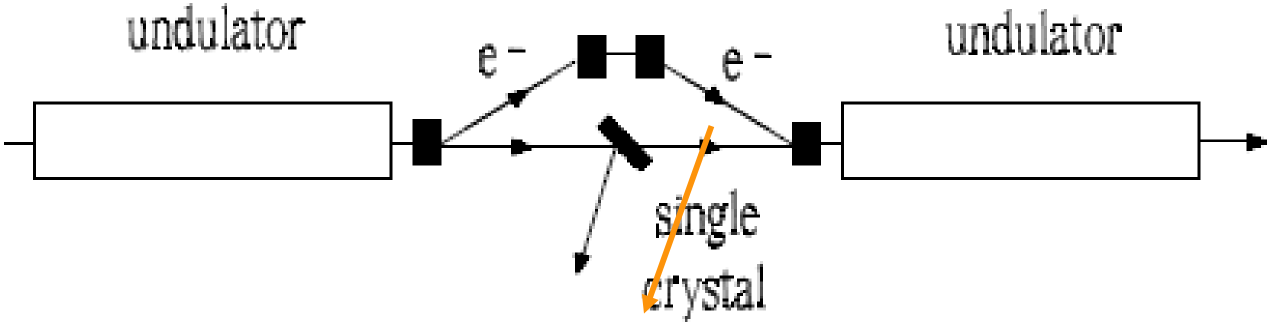
Working principle (V)

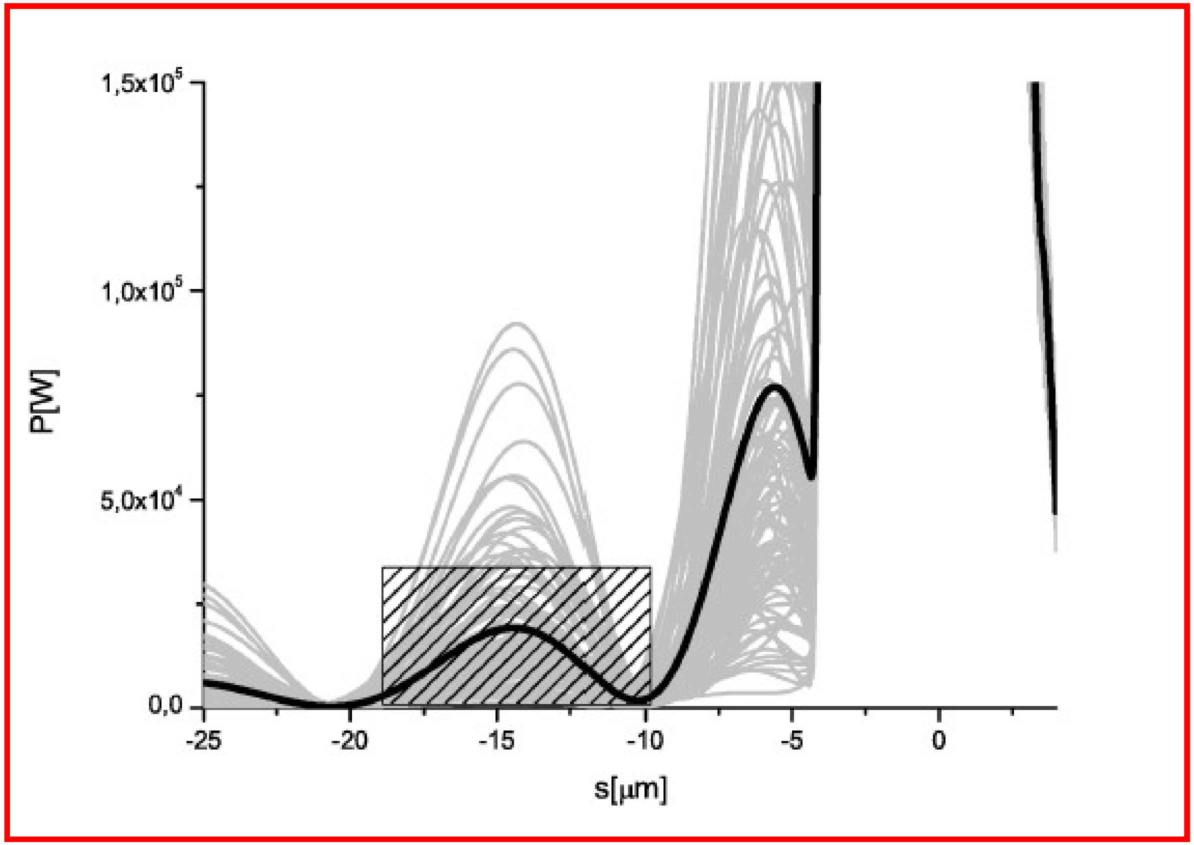
The single-crystal monochromator principle: time domain



Working principle (VI)

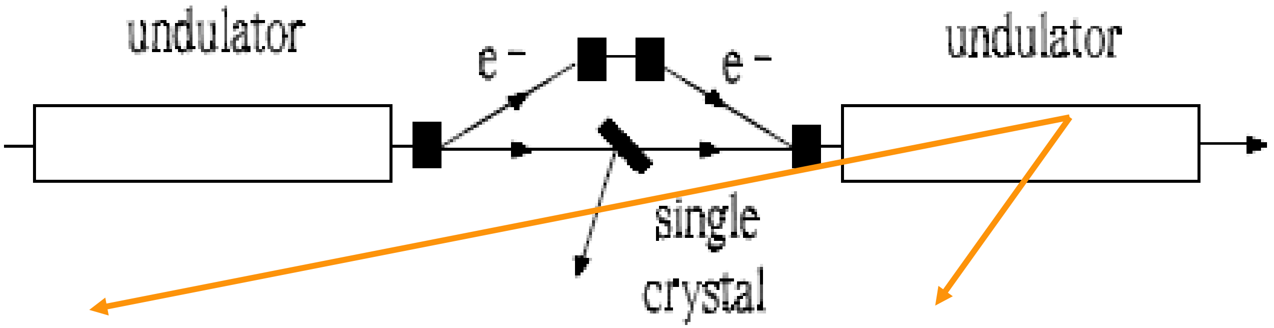
The single-crystal monochromator principle: time domain

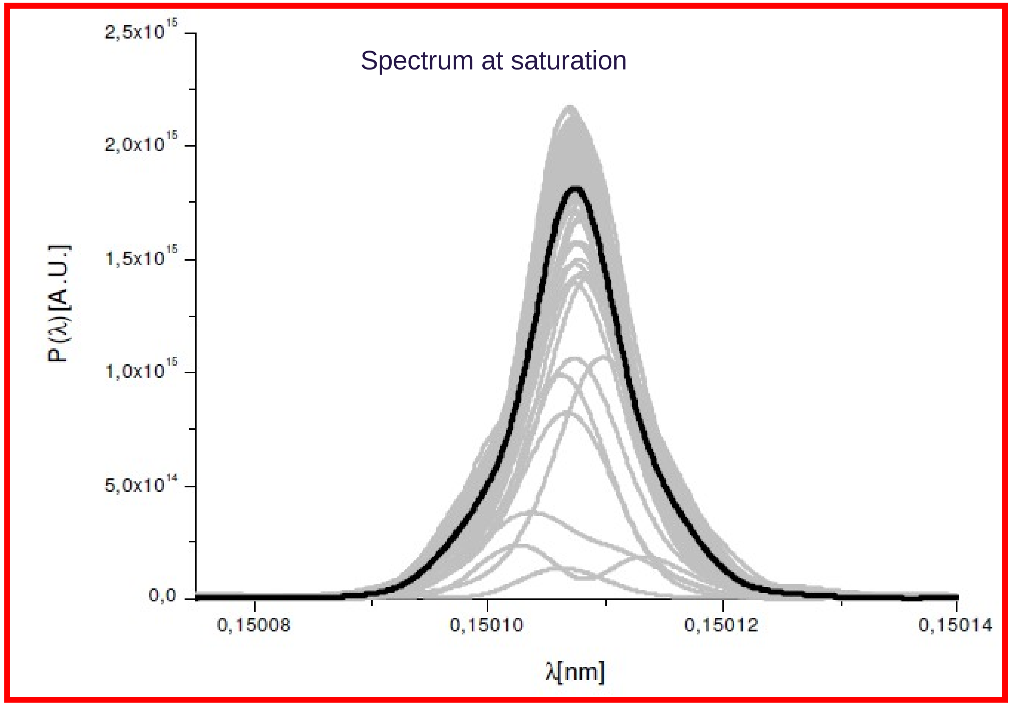


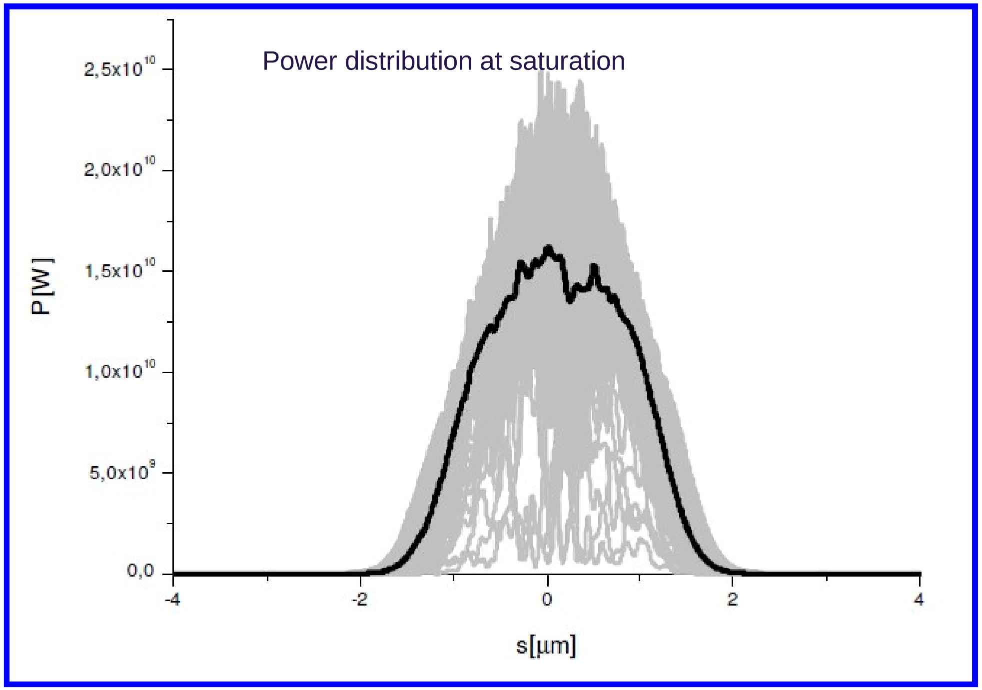


Working principle (VI)

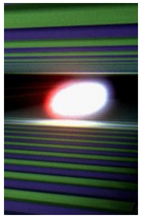
All that is left to do is to let the seed and the bunch into the radiator.
Seed is amplified up to saturation.




Spectrum at saturation

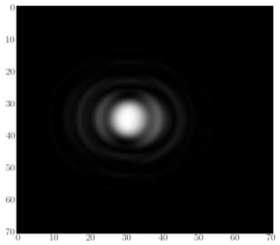

Power distribution at saturation

Spontaneous synchrotron radiation

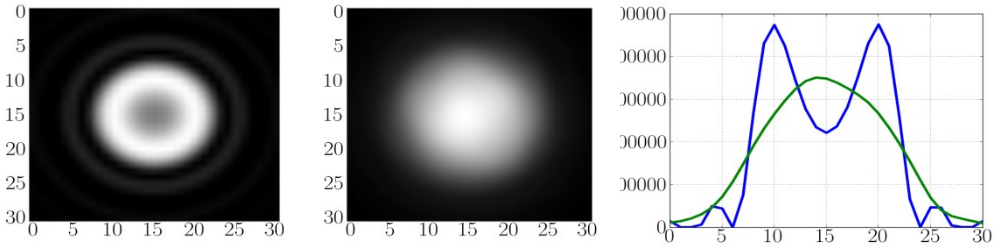


- Need for diagnostics, power loads and potentially science cases
- Numerical methods well understood, single particle solver provided by O. Chubar (SRWlib)
- Issues for xfel.eu: long undulators, narrow UR bandwidth, need to account for: electron optics, emittance, energy spread

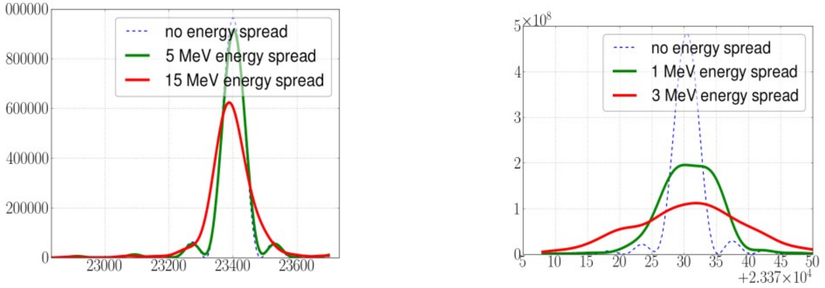
Effect of orbit distortion, flash



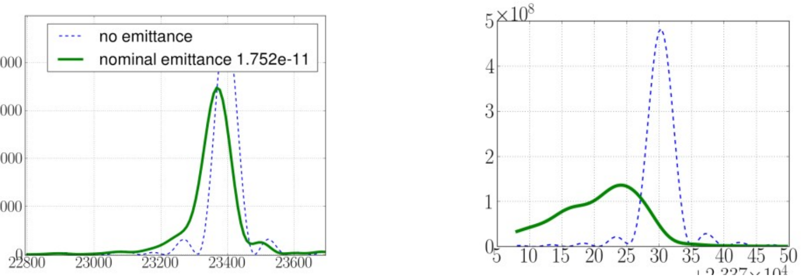
SASE1 (0.05nm), emittance effect on rad spot after mono



SASE1 (0.05nm), energy spread effect

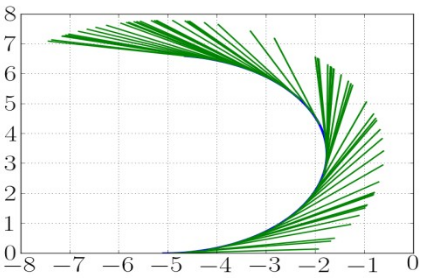


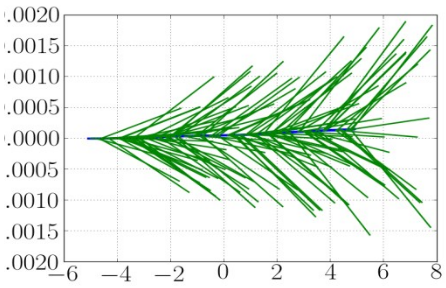
SASE1, emittance effect

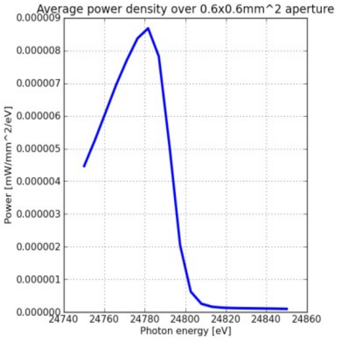


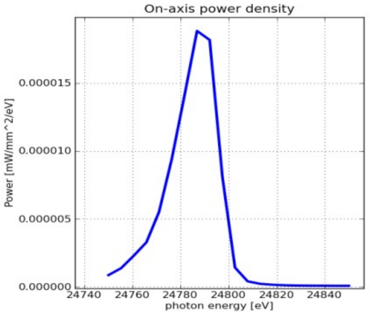
SR

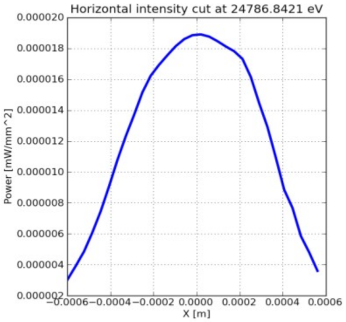
- SRW solver (O.Chubar and P.Elleaume, "Accurate and Efficient Computation of Synchrotron Radiation in the Near Field Region",EPAC-98)
- Based on the same e beamline model. Standard xframework components from which radiation can be caluclated: undulators with arbitrary polarization (analytical models and tabulated fields), quads, dipoles, sextupoles.
- Other solvers included (e.g. Monte-Carlo photon generator, bottom left)
- Solvers interchangeable
- Benchmarks are/have been done, as well as calculations for xfel with all effects (bottom right)
- SRW also allows for x-ray optics calculations. x-ray optic components (and particularly their placement) have not been standardized on xframework level,but direct access to appropriate srw functionality is always possible











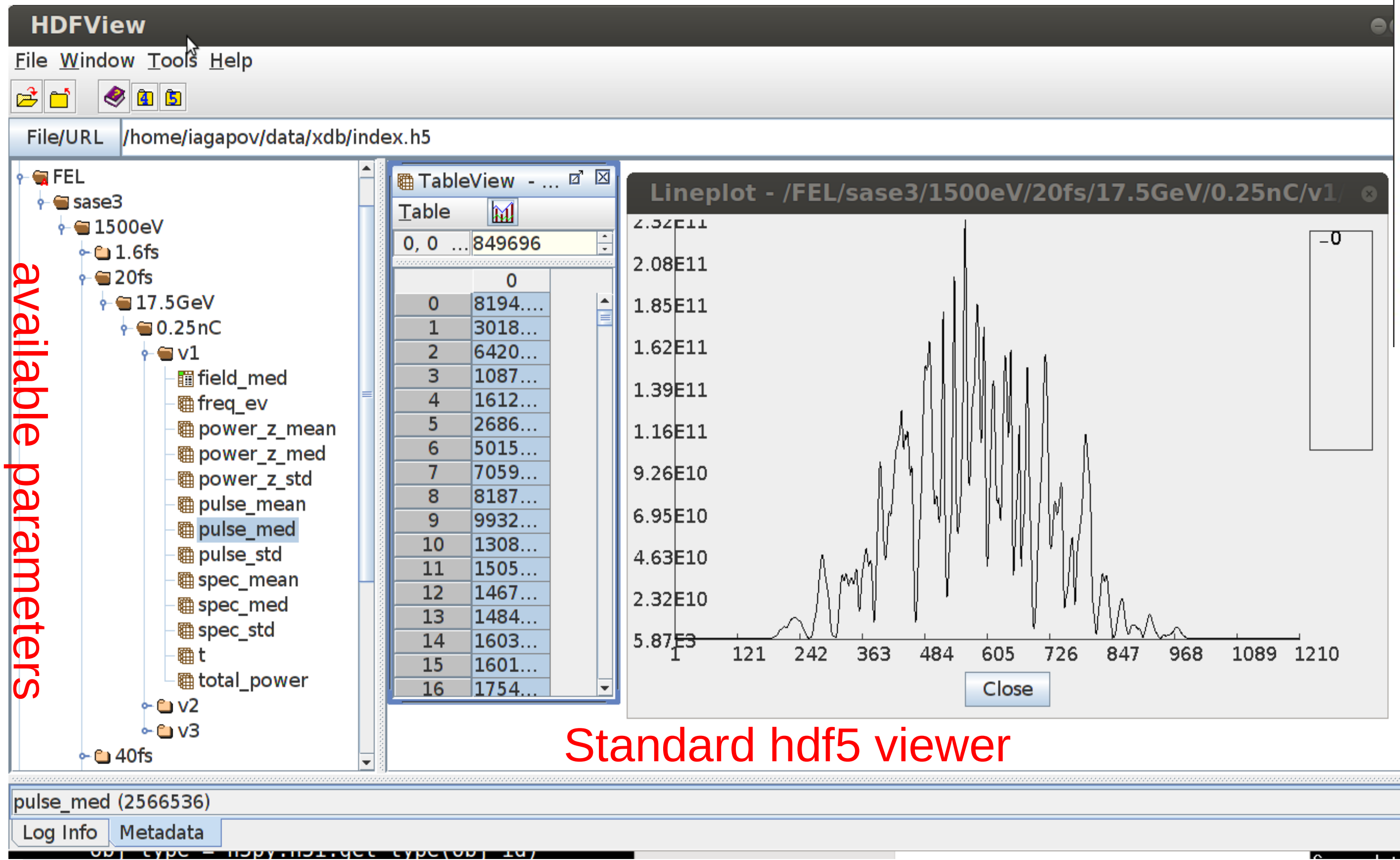
Overview of xcode

Xdb

- A tool to help users optimize their experiments

Self-consistent (includes input decks and run parameters)

- Runs (3d fields) → backup on storage?→statistics (hdf5) → index DB (hdf5)
- Command-line tools and python api
- Web interface possible (python fcgi prototype included)



/home/iagapov/data/xdb/index.h5

- FEL
  - sase3
    - 1500eV
      - 1.6fs
      - 20fs
        - 17.5GeV
          - 0.25nC
            - v1
              - field_med
              - freq_ev
              - power_z_mean
              - power_z_med
              - power_z_std
              - pulse_mean
              - pulse_med
              - pulse_std
              - spec_mean
              - spec_med
              - spec_std
              - t
              - total_power
            - v2
            - v3
      - 40fs

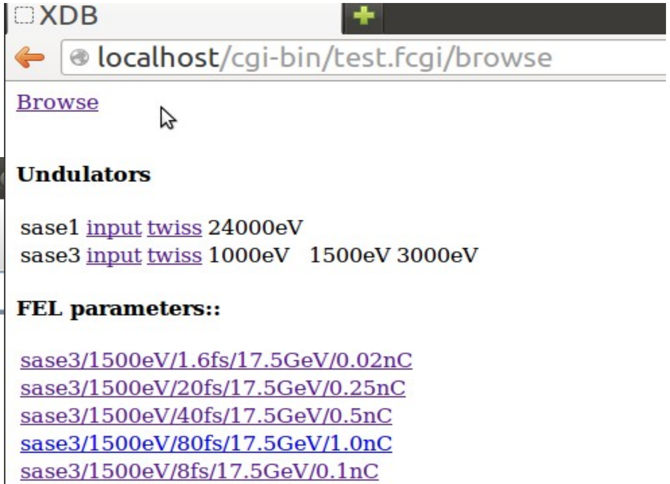
0, 0 ... 849696

	0
0	8194....
1	3018...
2	6420...
3	1087...
4	1612...
5	2686...
6	5015...
7	7059...
8	8187...
9	9932...
10	1308...
11	1505...
12	1467...
13	1484...
14	1603...
15	1601...
16	1754...

pulse_med (2566536)

available parameters

Standard hdf5 viewer



localhost/cgi-bin/test.fcgi/browse

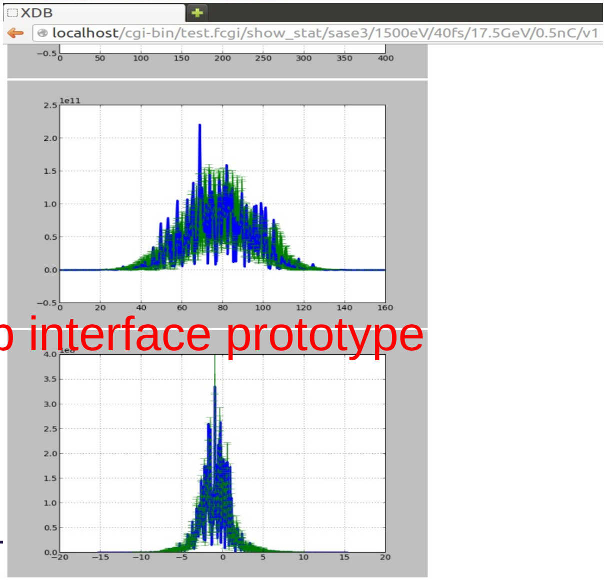
Browse

Undulators

sase1 input twiss 24000eV
sase3 input twiss 1000eV 1500eV 3000eV

FEL parameters::

sase3/1500eV/1.6fs/17.5GeV/0.02nC
sase3/1500eV/20fs/17.5GeV/0.25nC
sase3/1500eV/40fs/17.5GeV/0.5nC
sase3/1500eV/80fs/17.5GeV/1.0nC
sase3/1500eV/8fs/17.5GeV/0.1nC



localhost/cgi-bin/test.fcgi/show_stat/sase3/1500eV/40fs/17.5GeV/0.5nC/v1

web interface prototype

III/IV

Storage ring beam dynamics

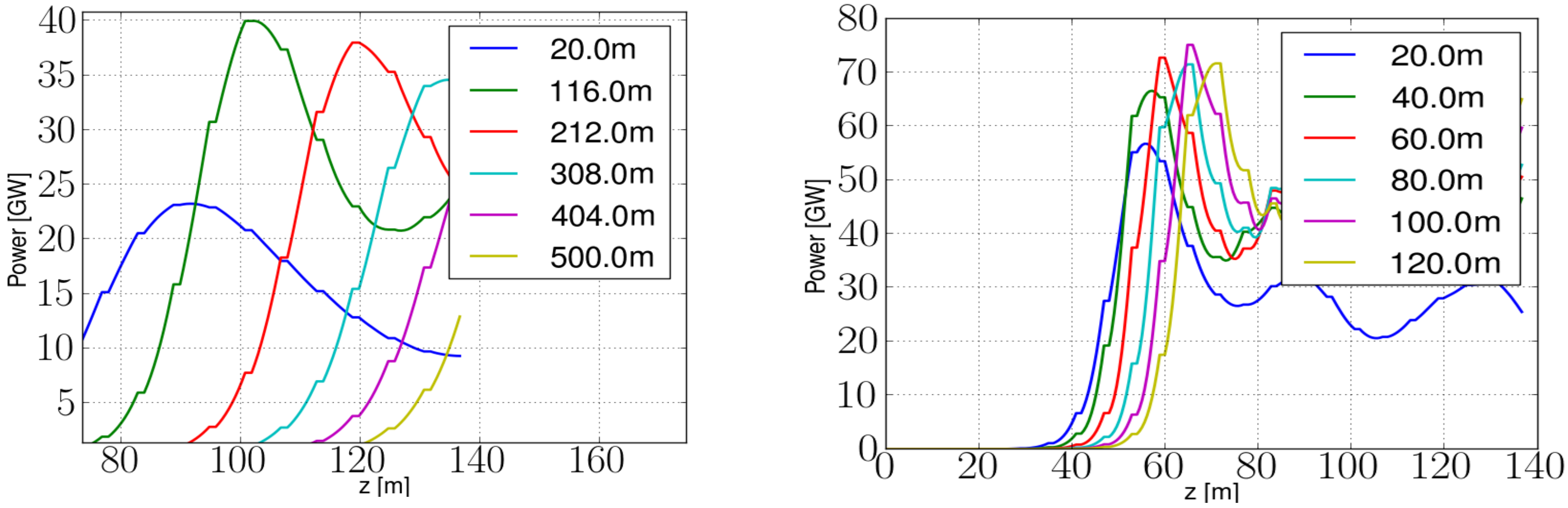
Original motivation

- FEL efficiency depends on the beta function, needed simple matching capabilities for optimization
- S. Tomin work on siberia2
- Potential interest in XFEL start-to-end simulations
- Started looking into petra3 beam dynamics recently

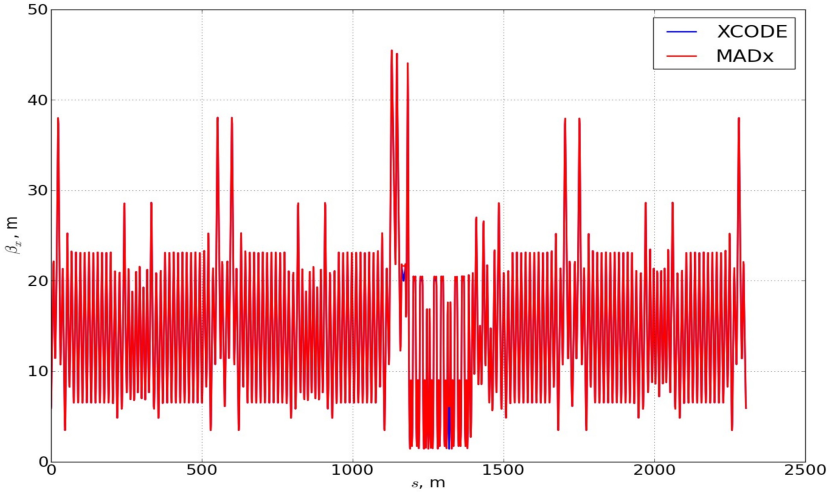
Petra3 parameters

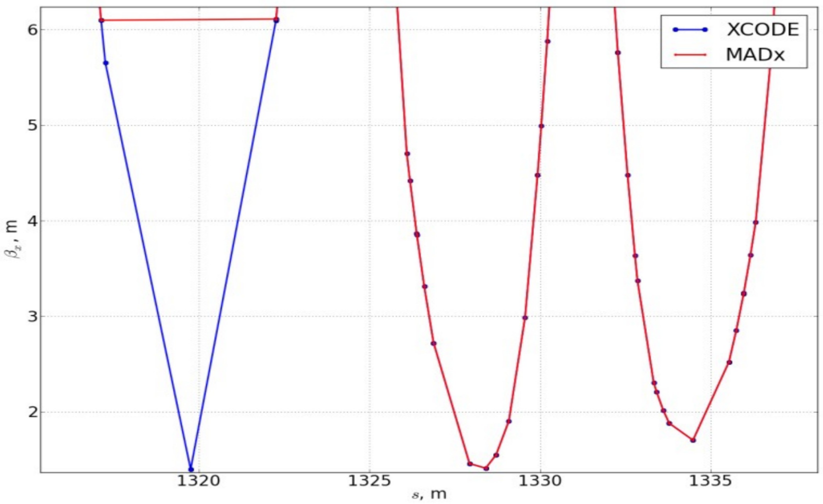
Parameter	**Value**
Beam energy	6 GeV
Circumference	2304 m
Emittance $\varepsilon_x, \varepsilon_y$	10^{-9}, 10^{-11}
Energy spread	10^{-3} (6MeV)
Bunch charge	20 nC
Bunch length	44ps or 13mm
Peak current	170A
Longitudinal damping time	10msec

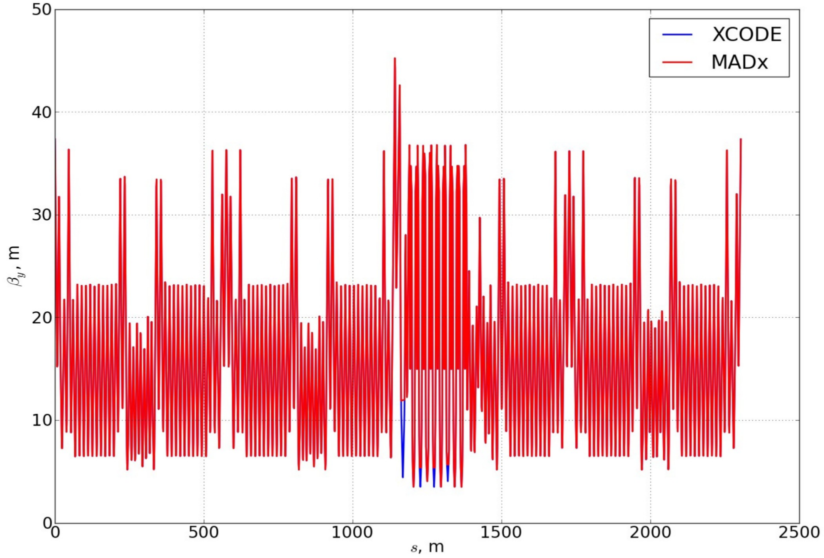
Dependence of fel power on beta function for XFEL

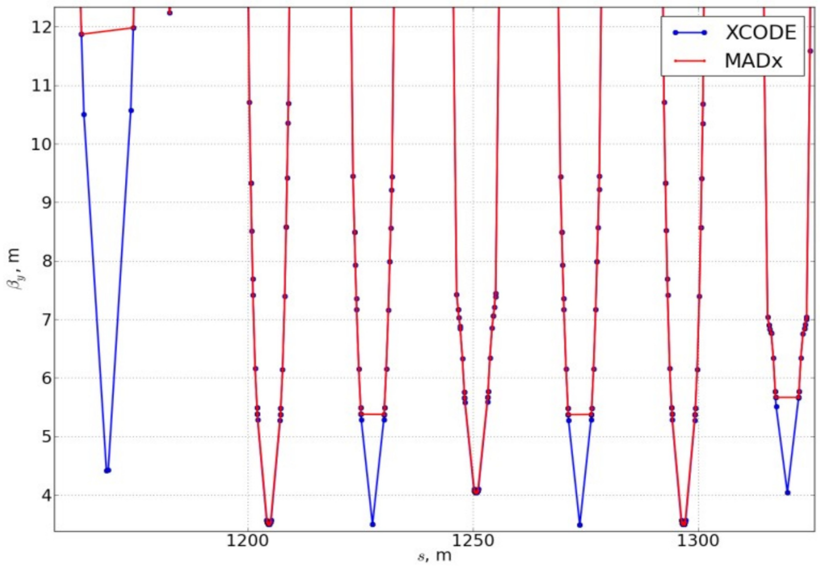


Linear optics cross-check with mad-x

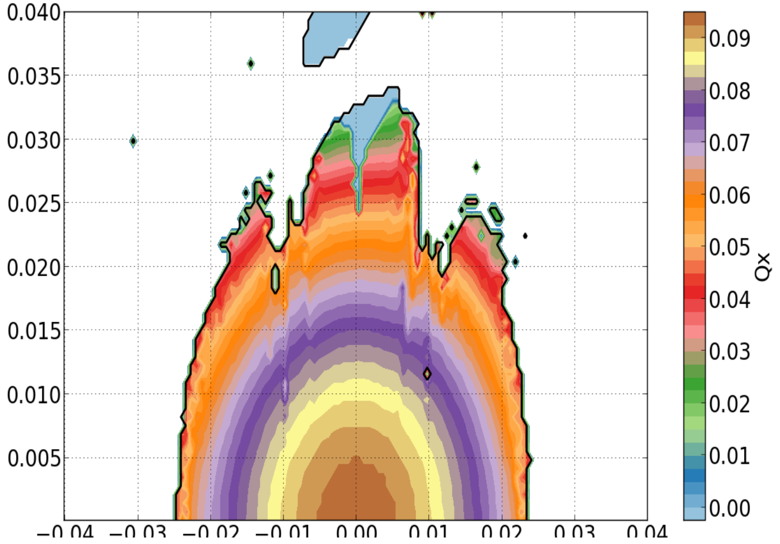


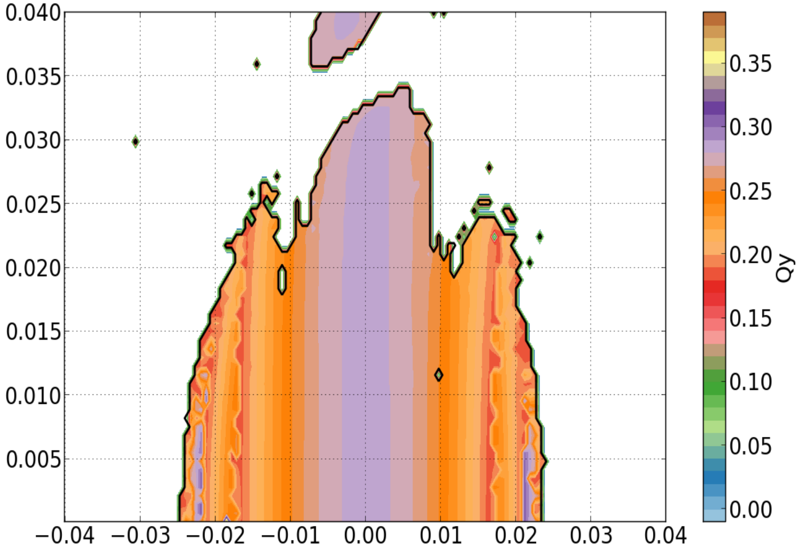


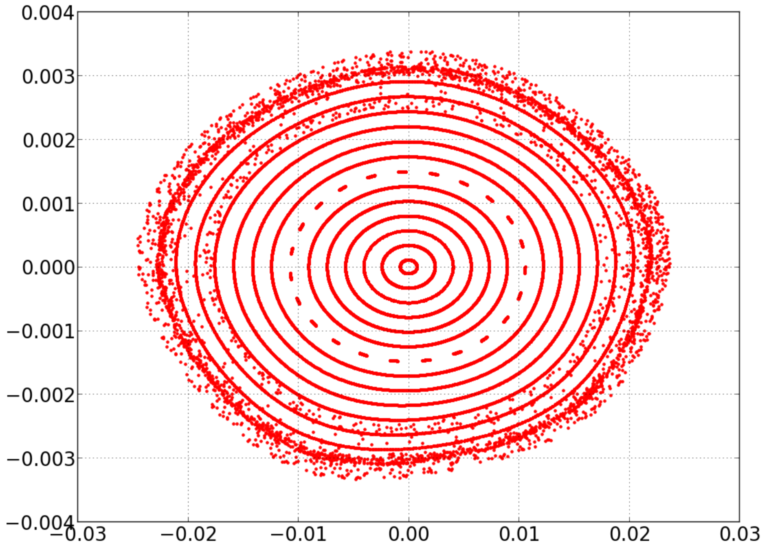


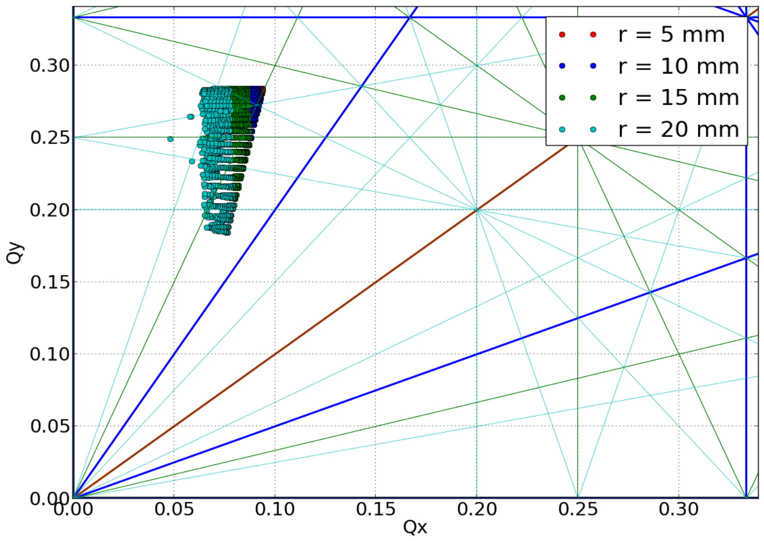


Nonlinear tracking: Petra3 without DWs and IDs

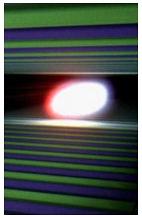


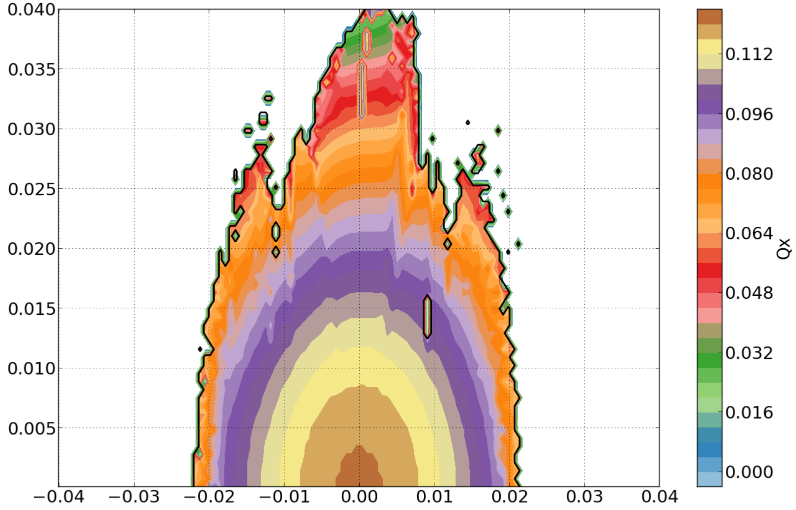


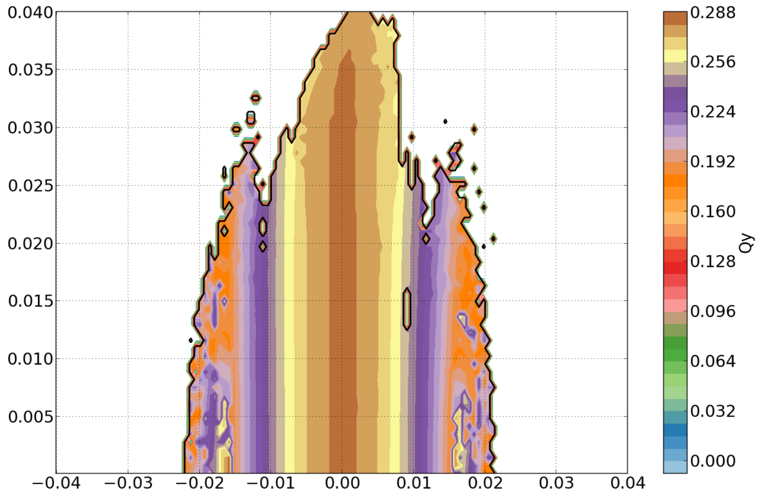


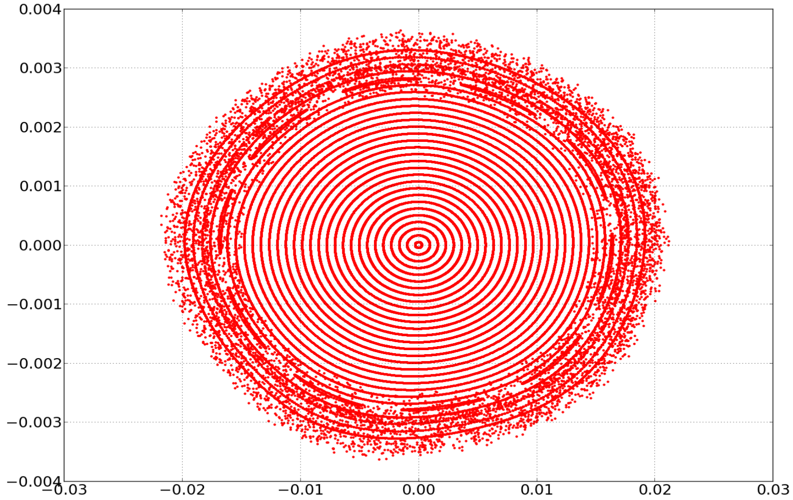


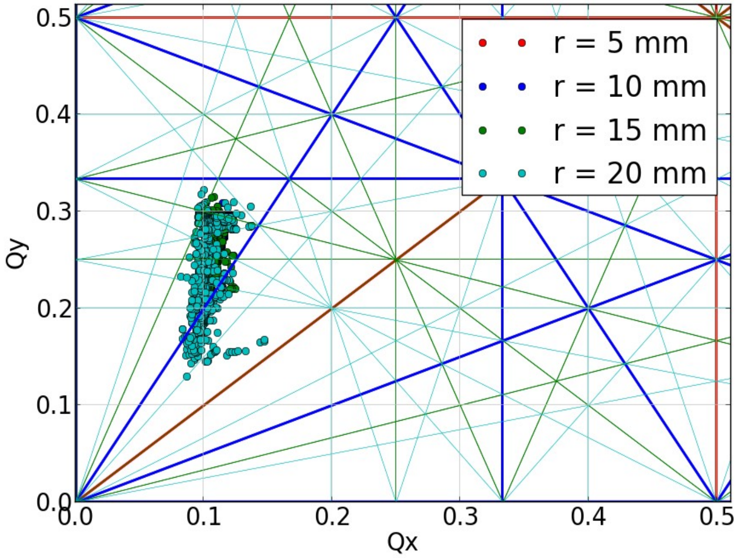
Petra3 with DWs and IDs



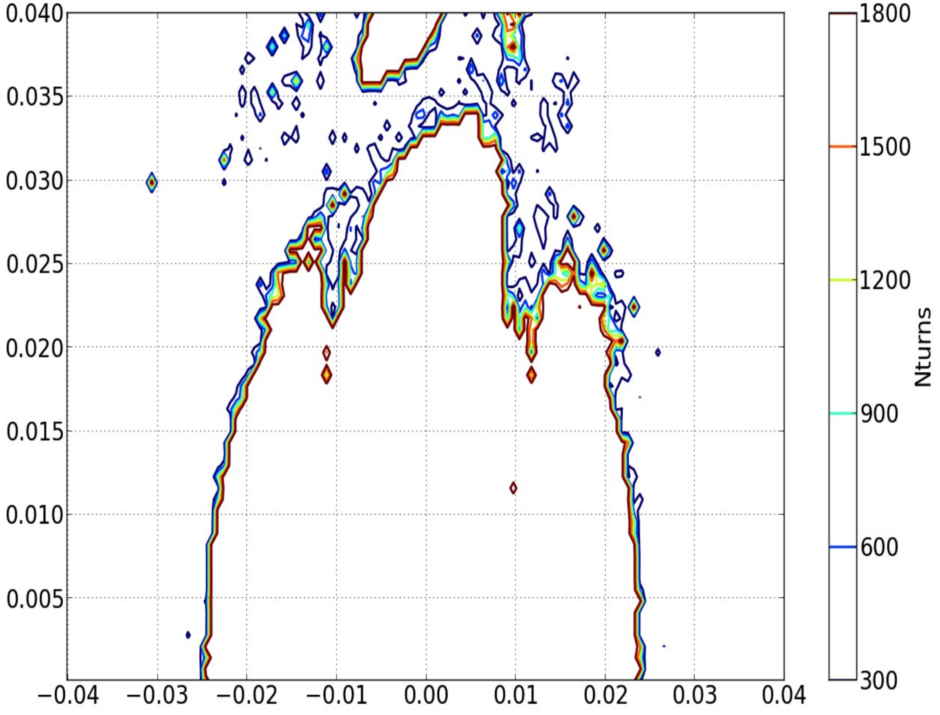


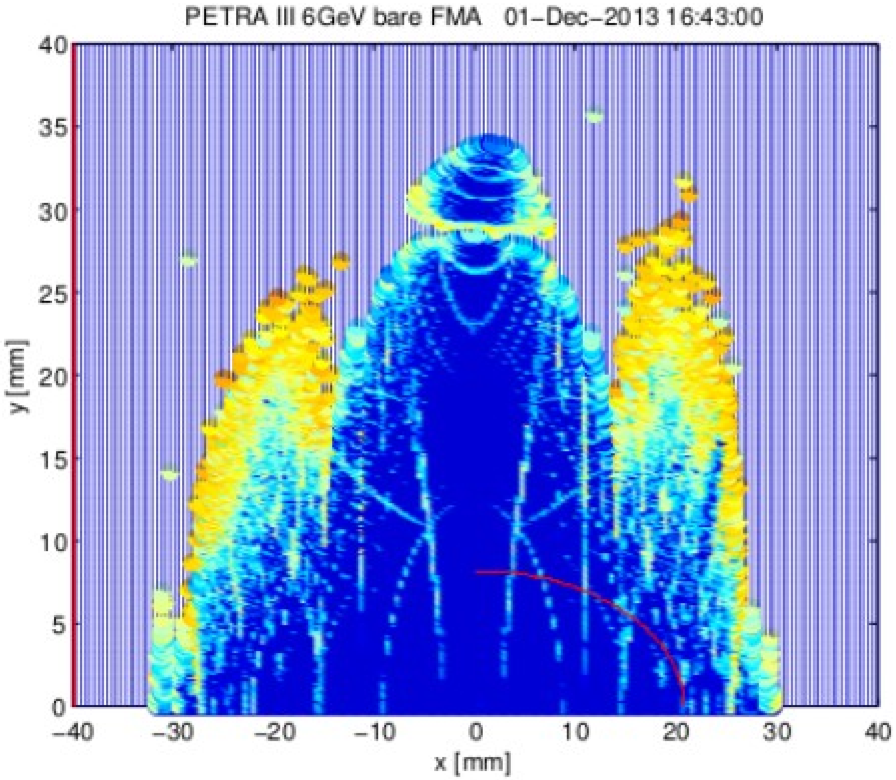






Dynamic aperture cross-check with SixTrack

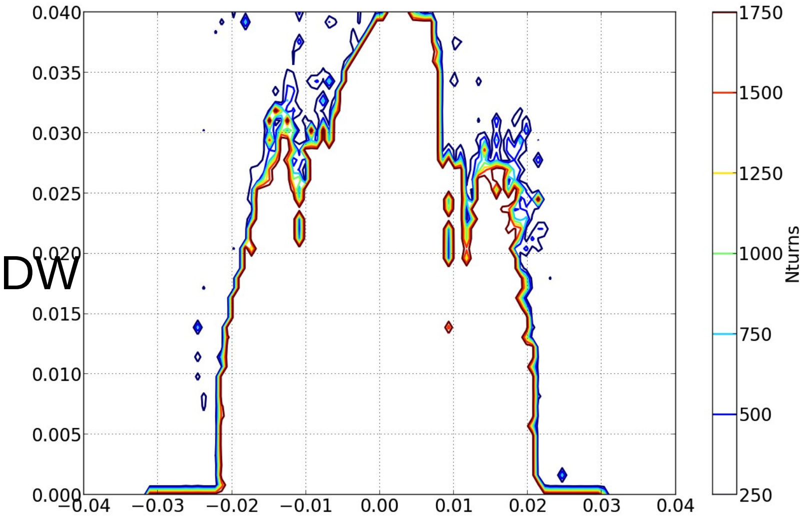




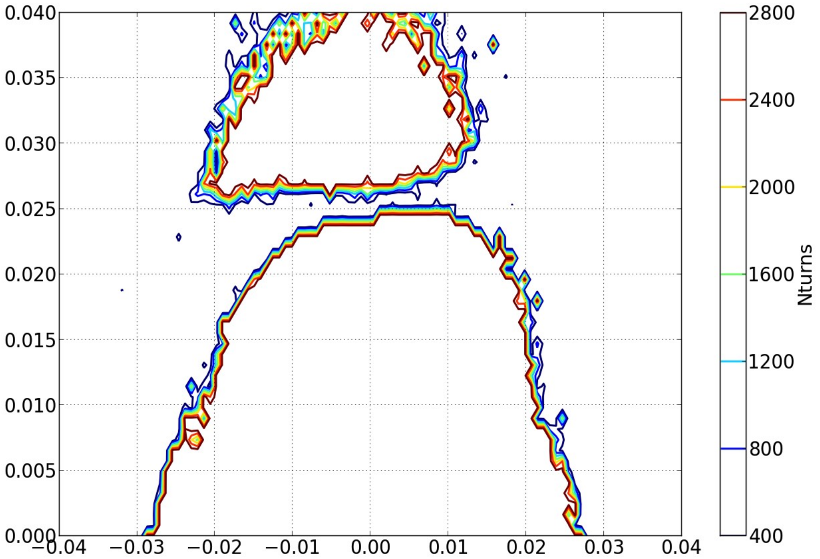
SixTrack (c/o Alexander Kling)

Calculations with various damping wigglers and insertion devices

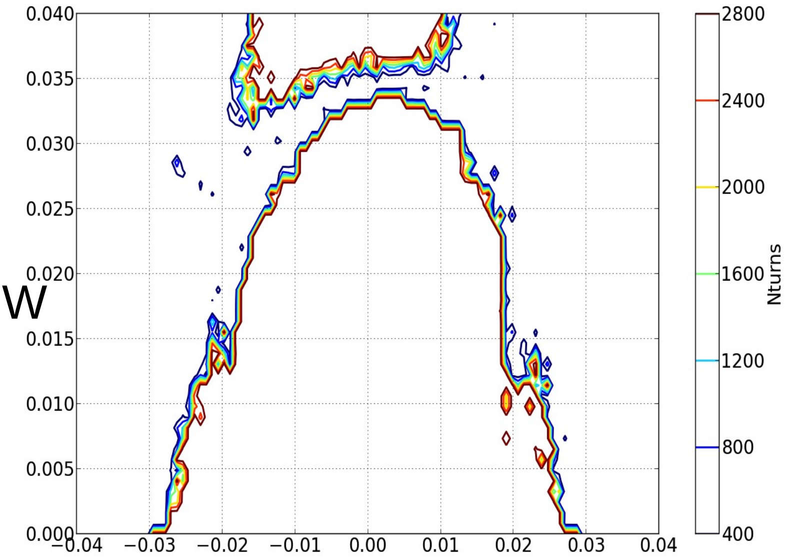
No DW



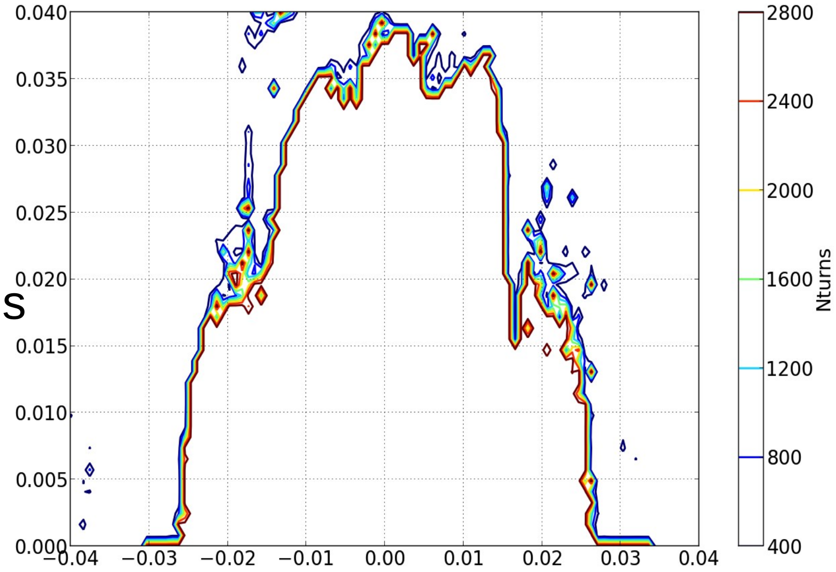
6 DW



10 DW

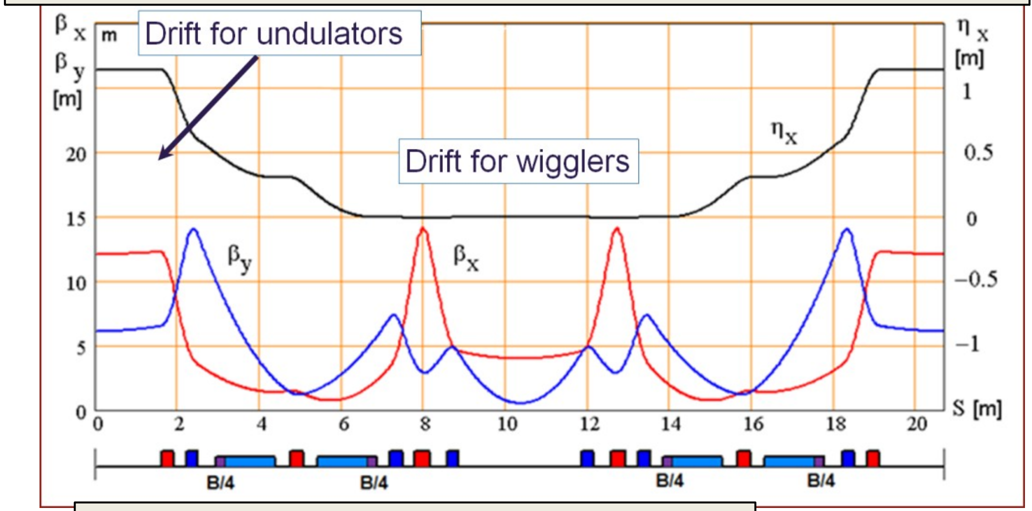


DW+IDs

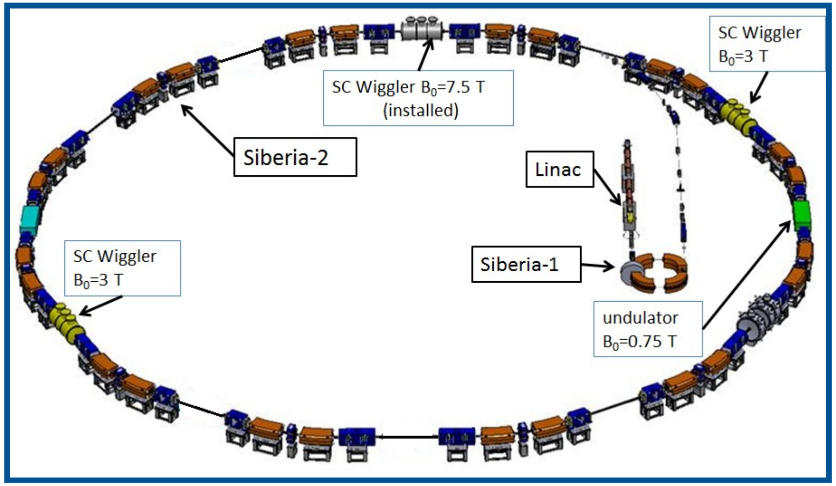


Example of DA calculations @ Siberia2

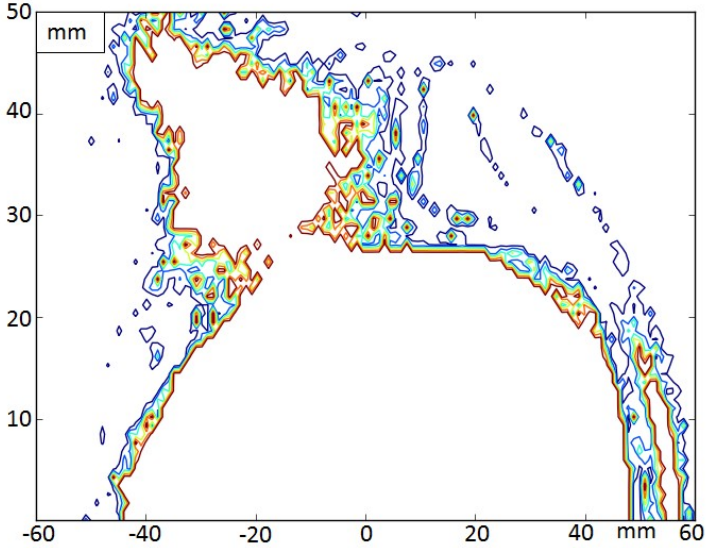
Optical functions of „standard“ structure (εx=98 nm rad)



Siberia-2 and proposed layout of insertion devices



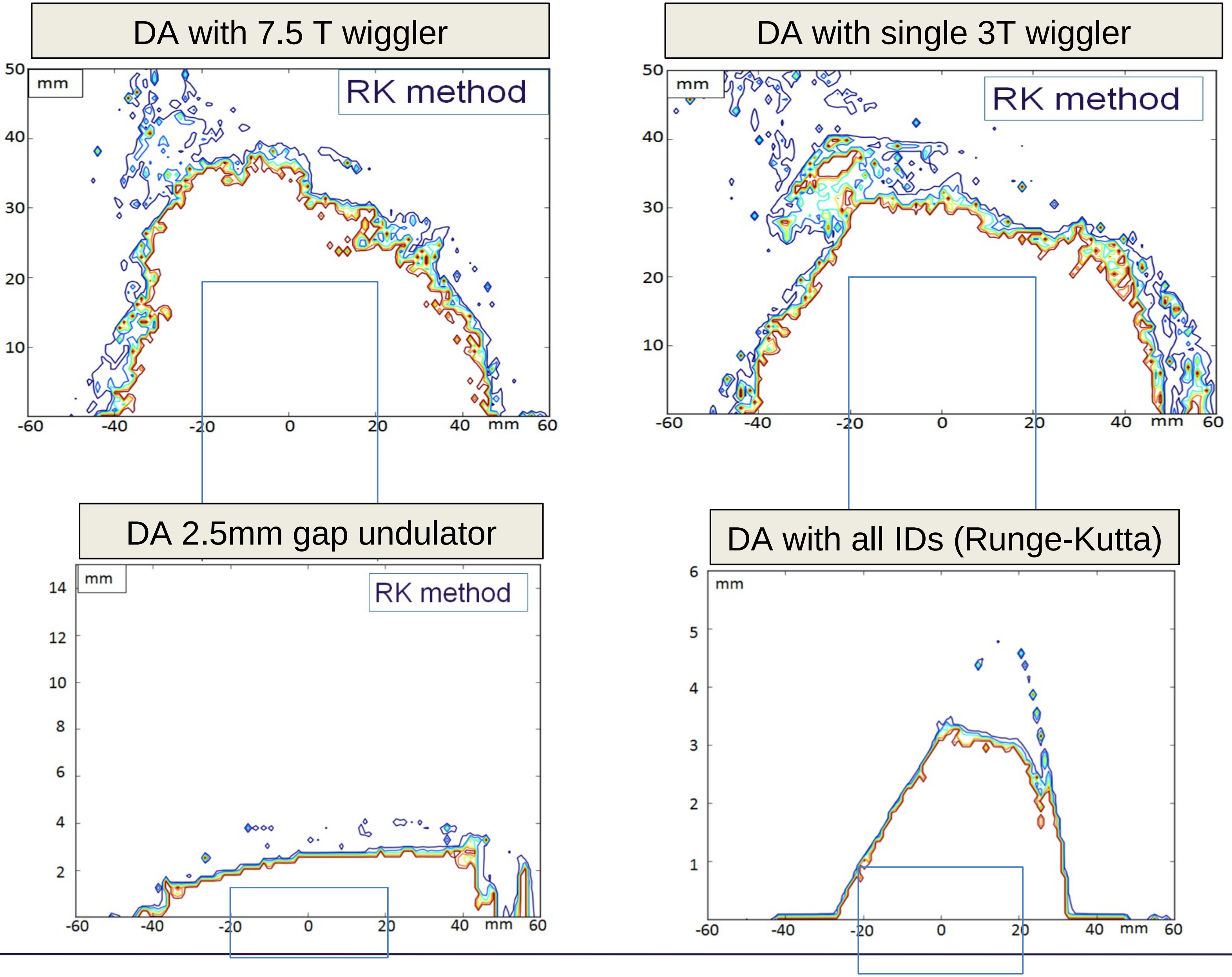
DA without ID



Main parameters of IDs

	Wiggler	Wiggler	Undulator
B_{max}, T	7.5	3	0.75
λ_{period}, mm	164	44	7
Field decrease ($k_x=2\pi/\xi$), ξ - , m	0.8	0.8	0.5
N_{period}	10	34	300
ε_{crit} radiation/ ε_1 (W=2.5 ГэВ), keV	30.7	8-16.4	ε_1=2
Deflection parameters	115	12.3	0.5
Spectral range, keV	20-150	5-40	2-7

Example of DA calculations @ Siberia2



DA with 7.5 T wiggler

DA with single 3T wiggler

DA 2.5mm gap undulator

DA with all IDs (Runge-Kutta)

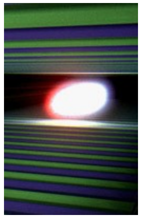
Current R&D

- Direction 1: introducing more storage ring related physics (IBS, Touschek,...)
- Direction 2: apparently there is heavy need in optimization for next generation storage rings. Current optimization methods are empirical and semi-empirical (MOGA) and require fast computation methods (e.g. DA). Currently looking into Lie methods to generate nonlinear one-turn maps for quick nonlinear dynamics calculations. Based on substantial body of theoretical work mostly in the 80s and 90s on using Lie maps for accelerator physics. Relative simplicity of polynomial manipulations in python makes this relevant

IV/IV

Longitudinal focusing

Linac FELs vs. synchrotron light sources



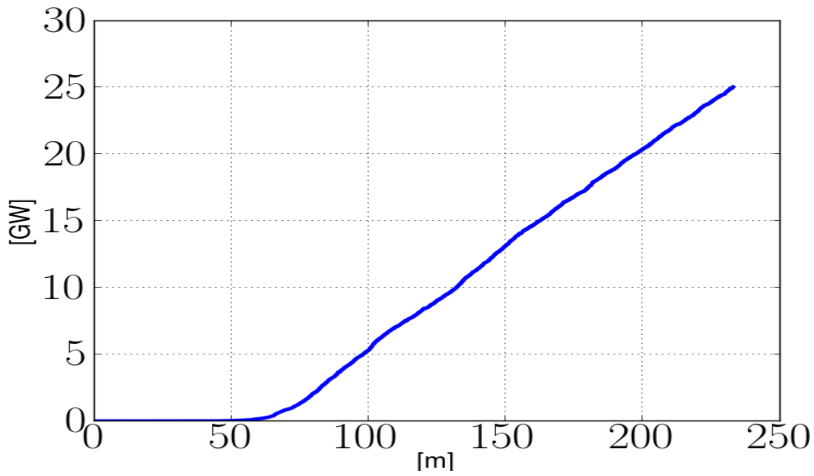
- FEL oscillators in storage rings historically studied in optical/IR . Abundance of dye lasers makes this less interesting now
- For x-rays mirror cavities a problem. High gain FEL in single pass.
- Linac pulse structure limited by RF. CW operation not easy. Thus linac FELs have pulsed photon flux(e.g XFEL.EU 2700bunches@10HZ)
- Beam Power normally wasted in a linac
- FEL requires extremely low emittances and high peak currents, which are possible with present gun technology (not achieved in storage rings)

FEL on a storage ring

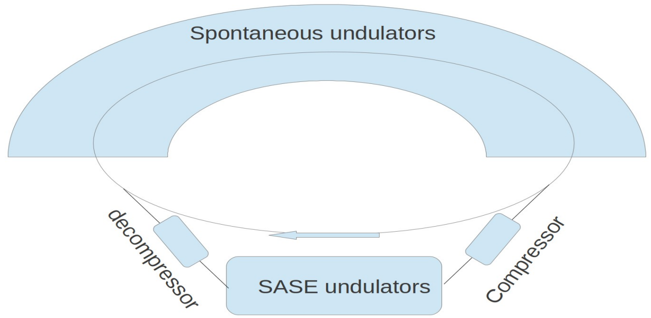
- Problems: instabilities and loss mechanisms grow rapidly with current (SASE being one such instability)
- Long sections not available
- FEL induced energy spread in addition to quantum diffusion. Translating deterministic energy modulations into energy spread
- All these make storage ring based FEL extremely difficult, although such studies have been performed

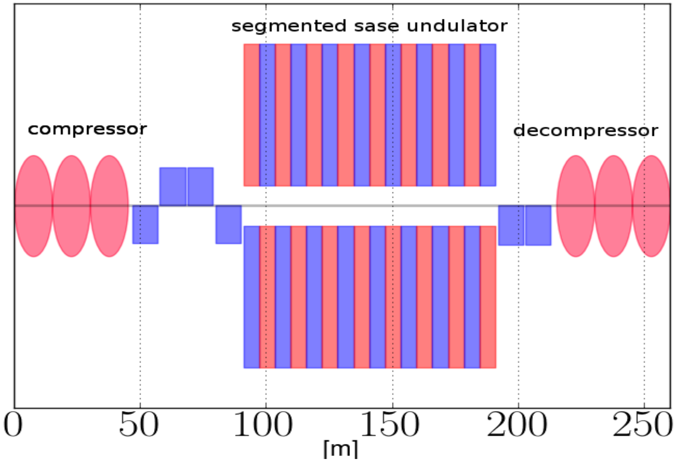
Longitudinal focusing

- One potential scheme to approach the necessary beam parameters might be additional compression at the insertion device



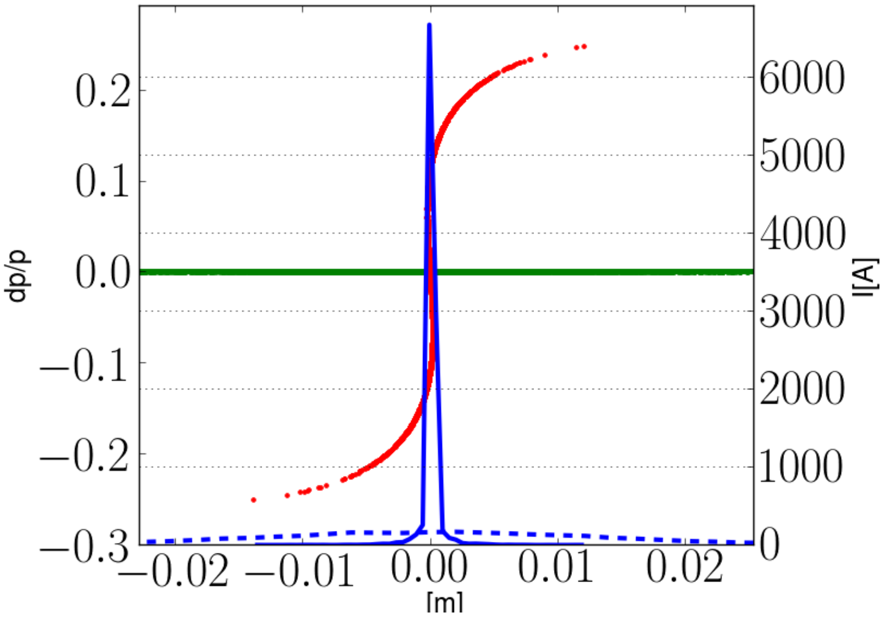
335 eV 50x compression
Petra3 emittance and bunch length parameters



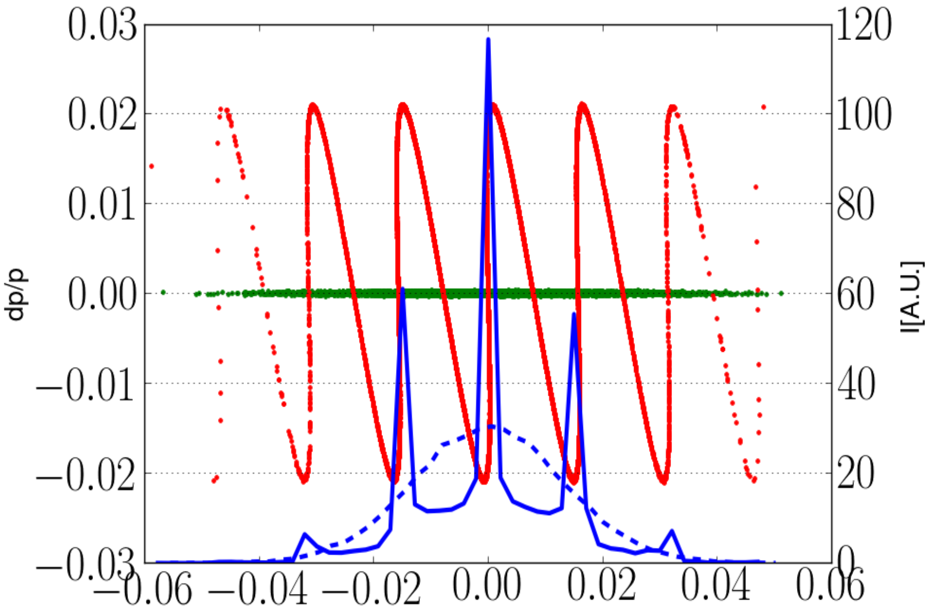


FEL on a storage ring

- From longitudinal dynamics perspective seems feasible (multi-turn map Taking into account energy loss and diffusion)



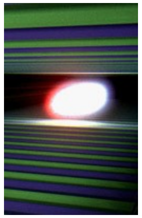
0.8 GHz



3.9 GHz

Required R'n'D

- Check feasibility with better emttance (e.g. USR parameters)
- Check equilibrium beam parameters
- Fit into ~20m undulator
- Look into optics (very large momentum acceptance, dispersion cancellation) , DA



Summary

- Developed a python framework supporting beam optics, SR, and FEL calculations
- Extensively using it to characterize radiation parameters at XFEL.EU
- Performed extensive charged particle optics module cross-checks

and are aiming at extending its usage for light source RnD