



Xcoll
Xboinc
Xdyna

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ABP Technical Meeting on Large Simulation Codes, 19/10/2023

Xcoll

Everything you need for your collimation simulations in Xsuite

Design Philosophy

- **Standardisation:**

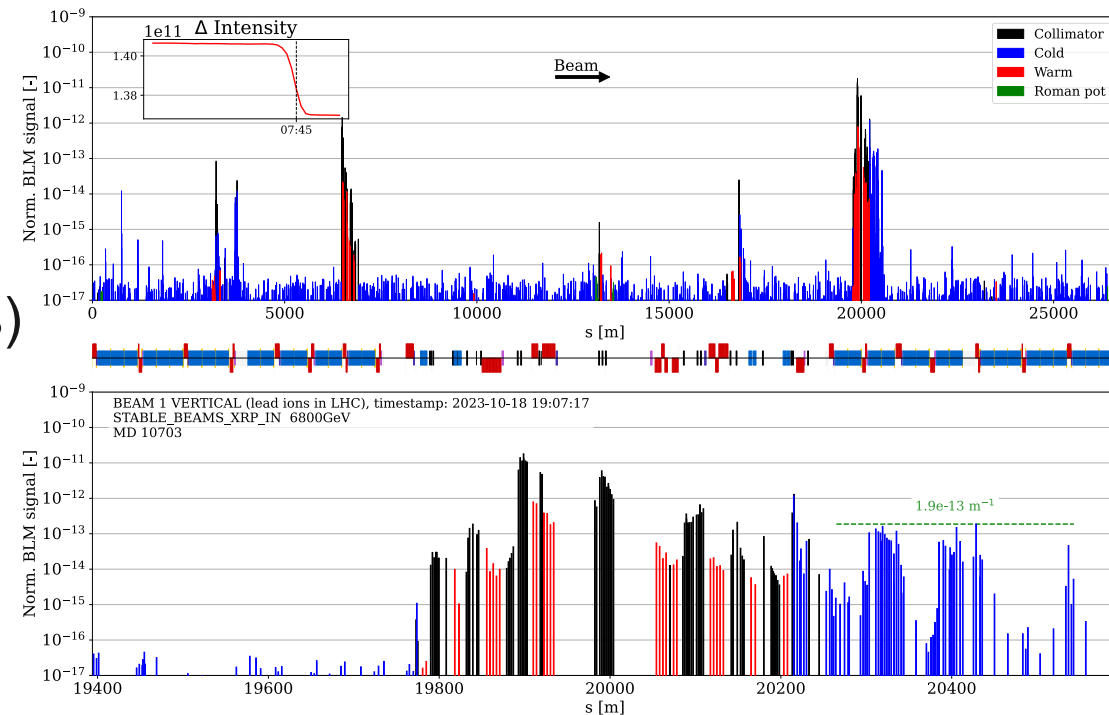
- common approach for easy comparison between different simulation setups and measurement
- e.g. direct integration with recent lossmaps tool

- **Flexibility:**

- user-friendly modularity stimulates autonomy (not dependent on developers for small changes)
- while guaranteeing robustness and reliability

- **Maintability:**

- code readability and documentation is a must to ensure future-proofing code development
- robust and encompassing test suite

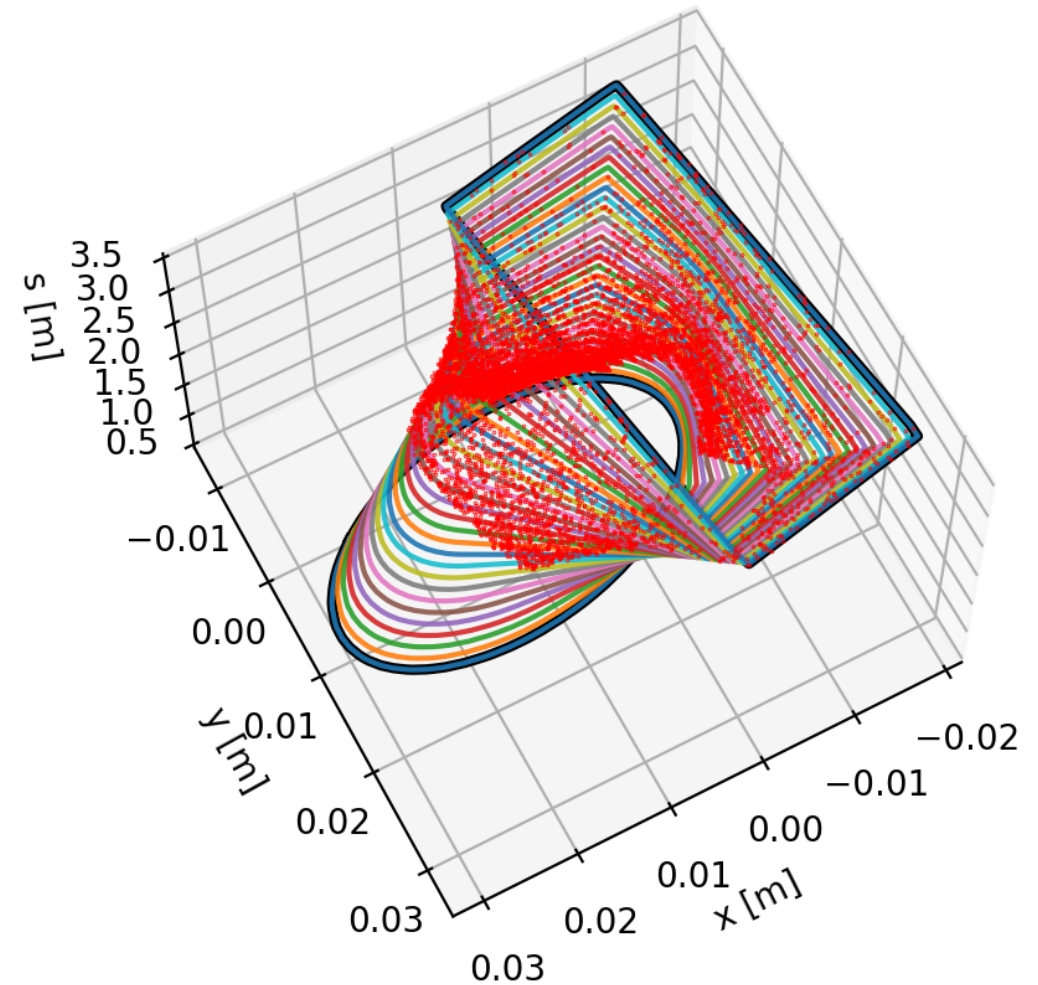
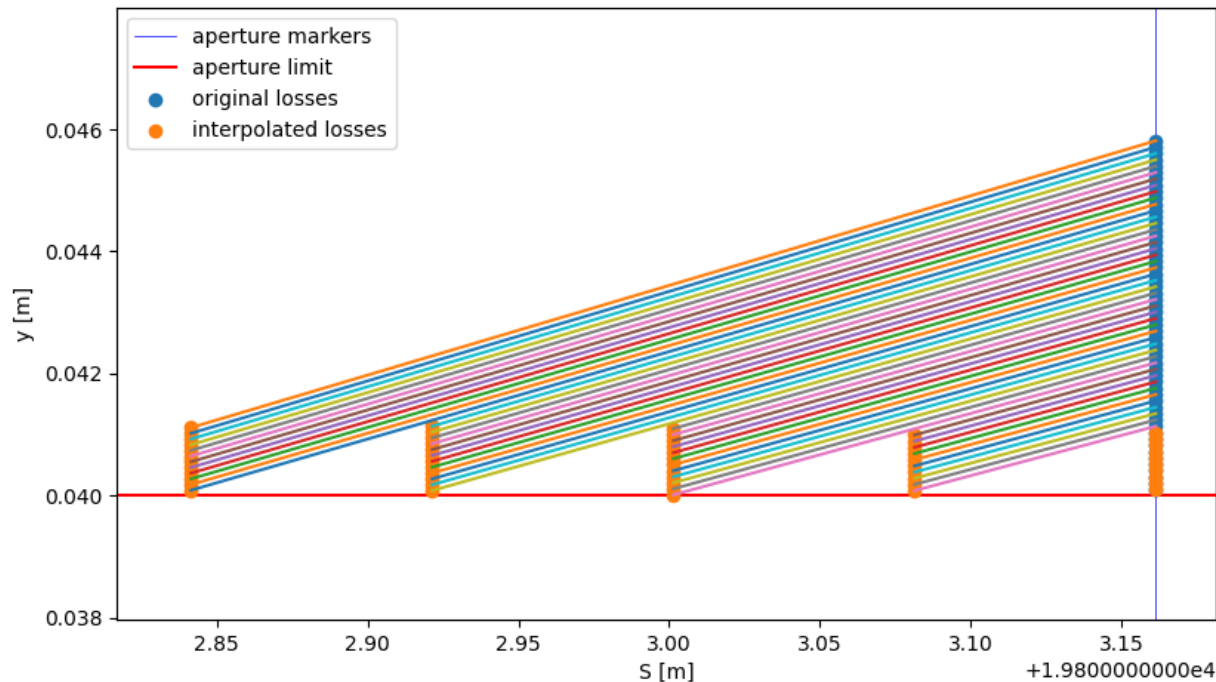


Features

- **Collimator installation:** special care for consistency (cryo tank, entrance markers, aperture, ...)
- **Collimator settings management:** CollimatorDatabase (YAML) \Leftrightarrow BeamElement
- **Initial distributions** (Xpart): annular halo, pencil beam (betatron and/or off-momentum), ...
- **Scattering Engines:** Everest (native), FLUKA (via FlukaIO), Geant4 (via collimasim+BDSIM)
- **Aperture interpolation** (Xtrack): consistency of aperture model along the lattice
- **ImpactTable:** precise logging of different scattering interactions
- **Loss Map:** longitudinal histogram of losses along the lattice
- **RF Sweep:** realistic modelling of off-momentum loss-maps

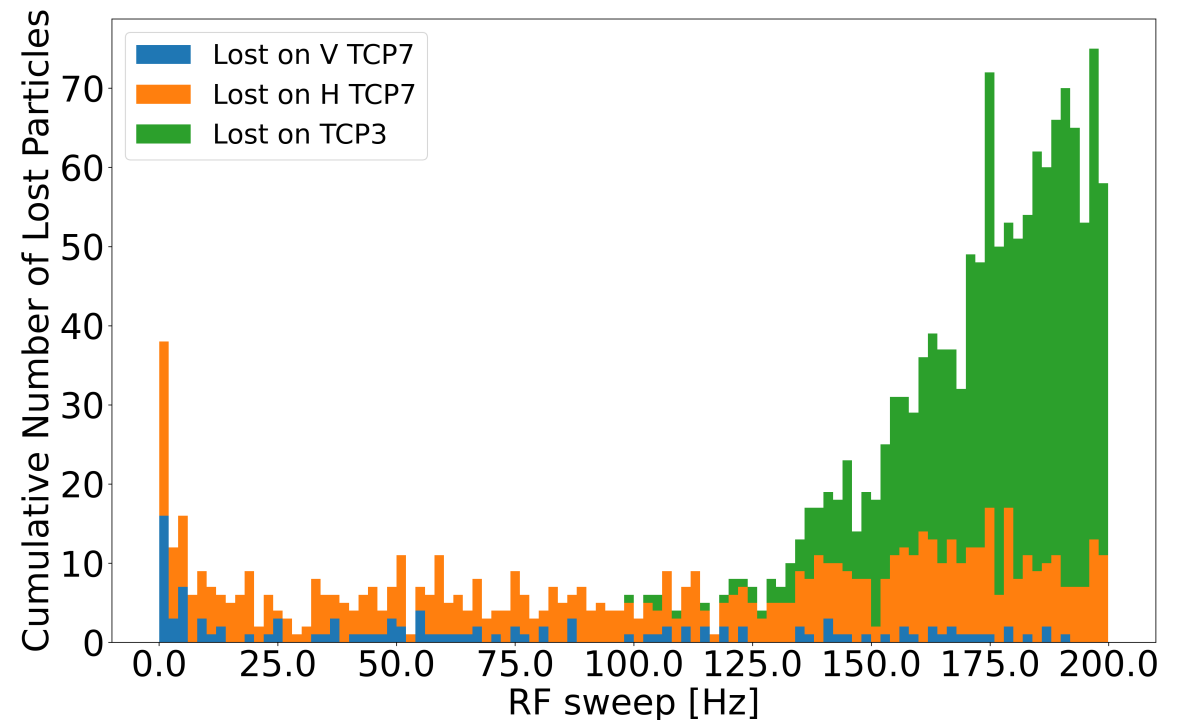
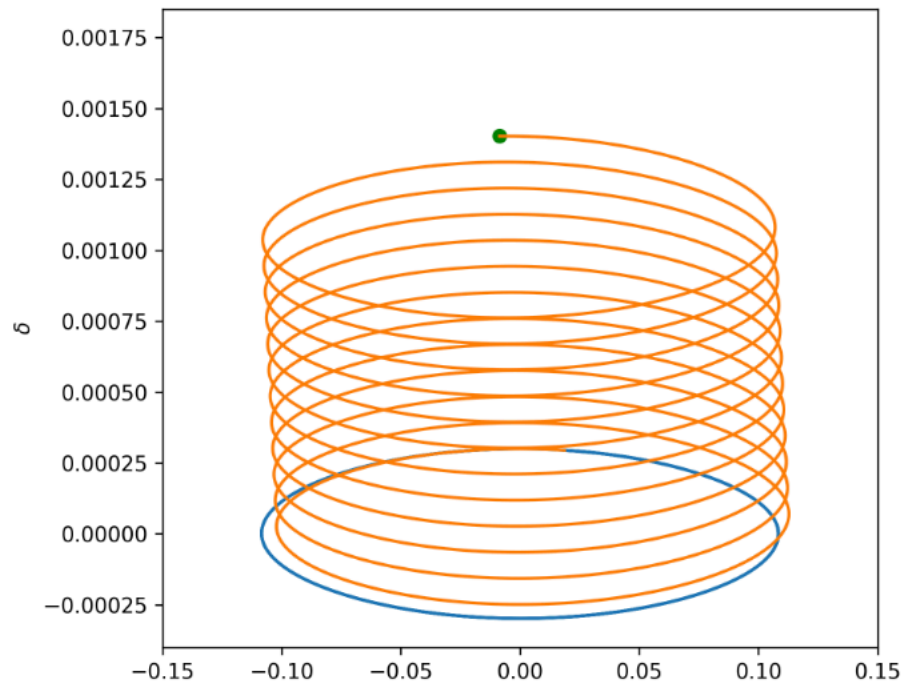
Aperture Interpolation

- Aperture markers can be limited to locations where aperture changes (for CPU efficiency)
- But need precise arbitrary resolution => **backtrack**
- **Interpolation** between different aperture types



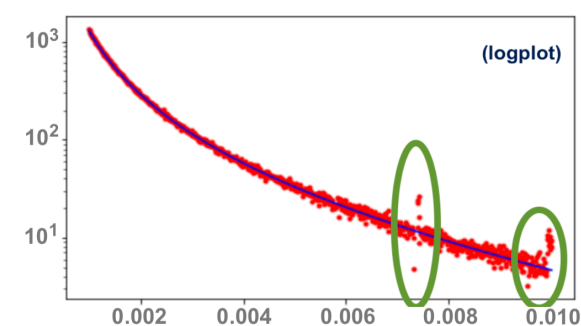
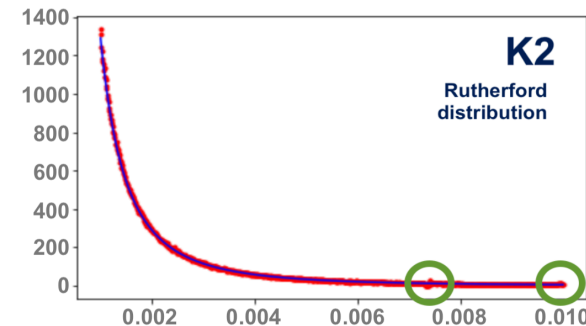
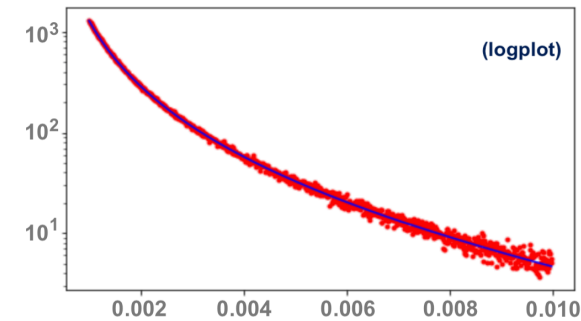
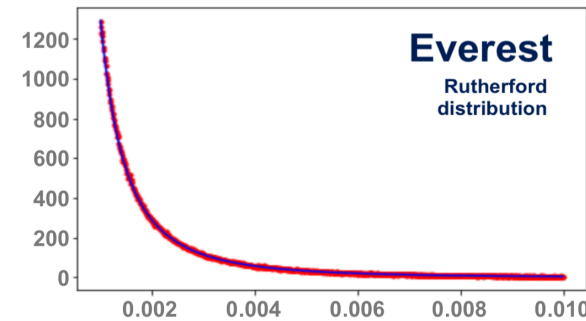
RF Sweep

- Sweeping frequency of RF cavities moves separatrix up/down along delta
- In simulations, particles are assumed synchronous to longitudinal reference trajectory
=> need to shorten/lengthen trajectory to simulate sweep
- See <https://www.overleaf.com/read/kcgwmgwrfwhw> for details



Everest

- **Native C** implementation (translated from FORTRAN)
- **Speed gain** of factor ~6 compared to K2 (single CPU)
- Low-level control exposed to user (e.g. tilts) (**NEW**)
- Rutherford random generator improved
- Code **readability** and logic flow improved
- **OpenMP-compatible (NEW)**
- Impact table improved
- Small updates/improvements to physics, like MCS (WIP)



Example application:

Betatron cleaning during Ramp

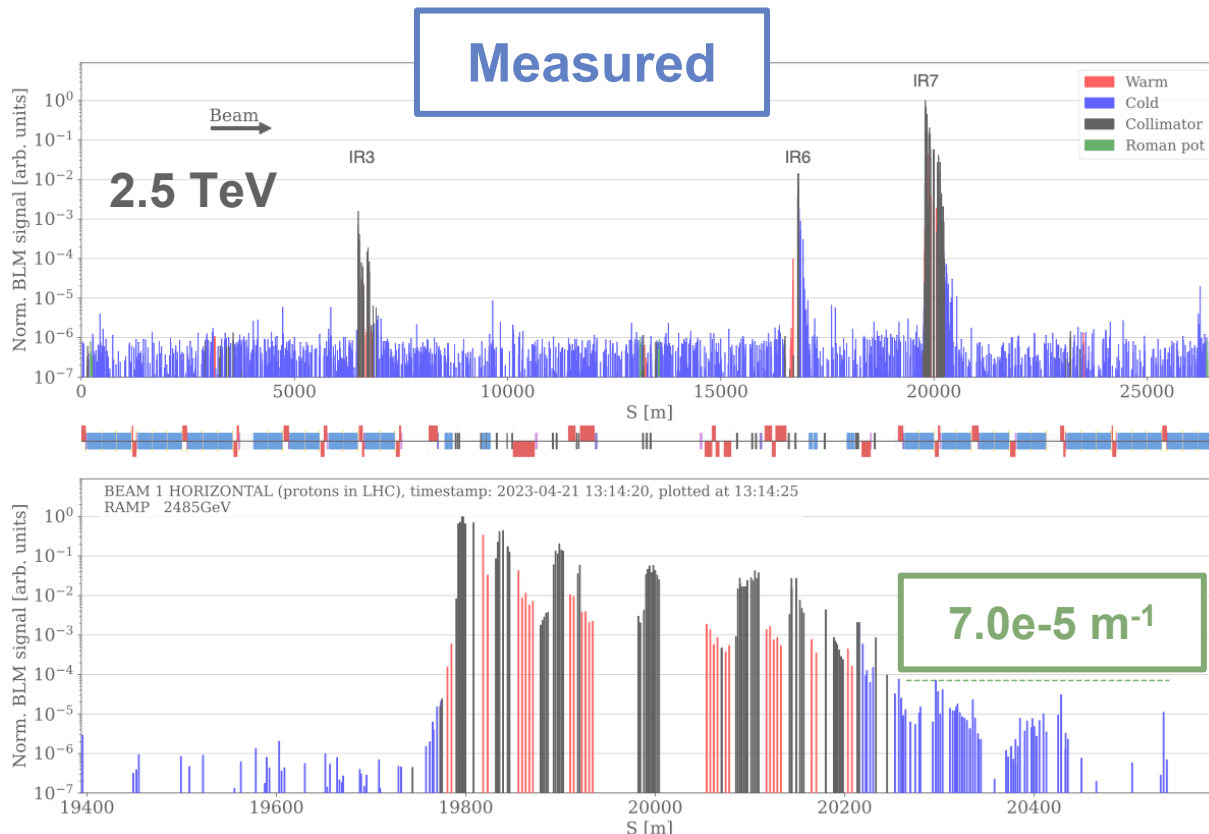
- **Good qualitative agreement** between measurements and simulations
 - Highest losses in IR7: similar **loss pattern**

Cleaning inefficiency simulations

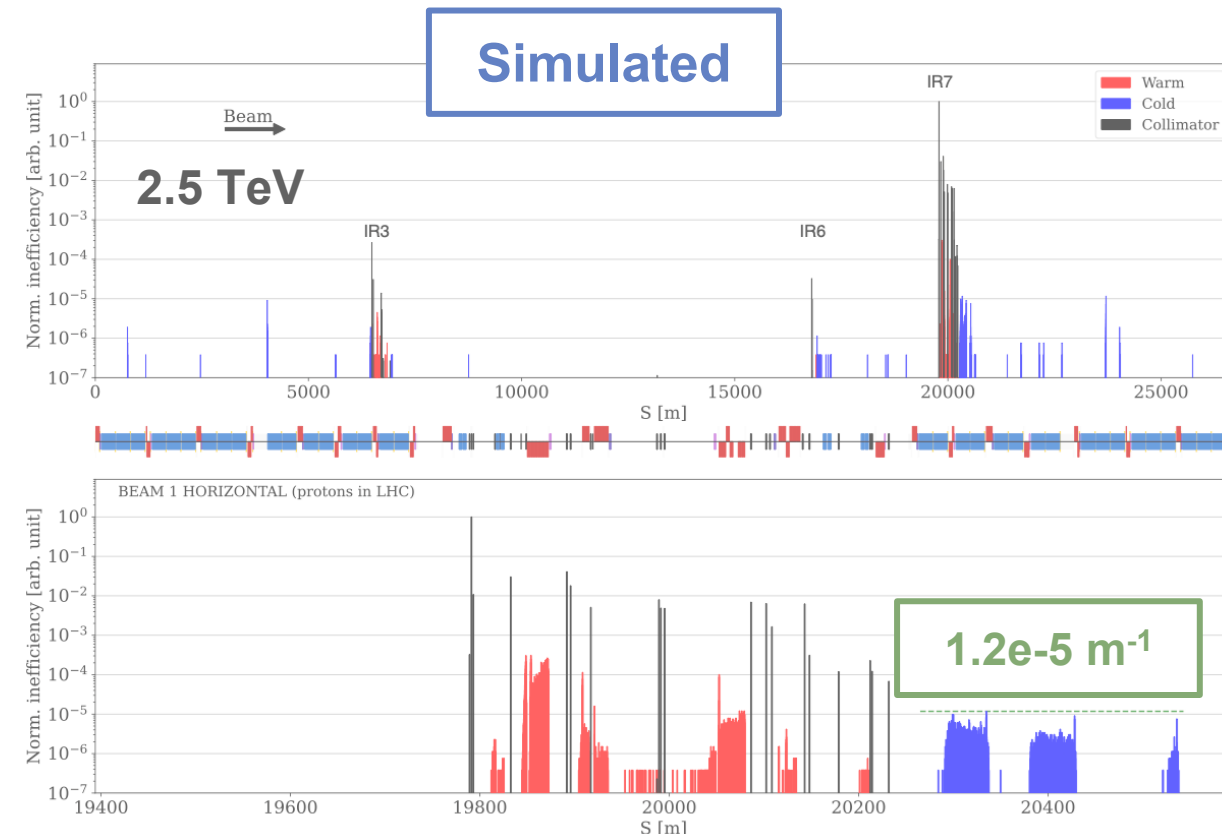
$$\eta = \frac{N_{\text{loc}}}{N_{\text{tot}} \Delta s}$$

where N_{loc} the local losses over distance Δs and N_{tot} is the total number of losses in the collimation system

Measured



Simulated

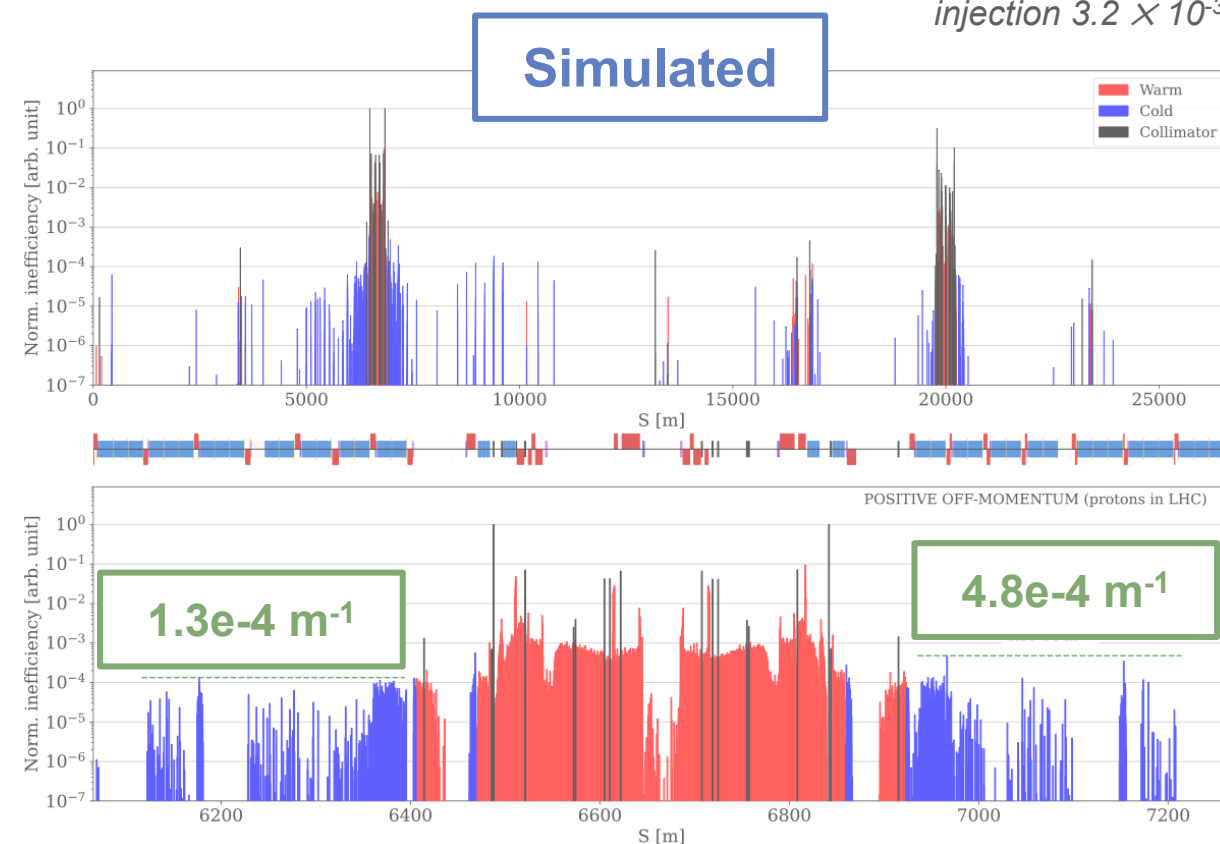
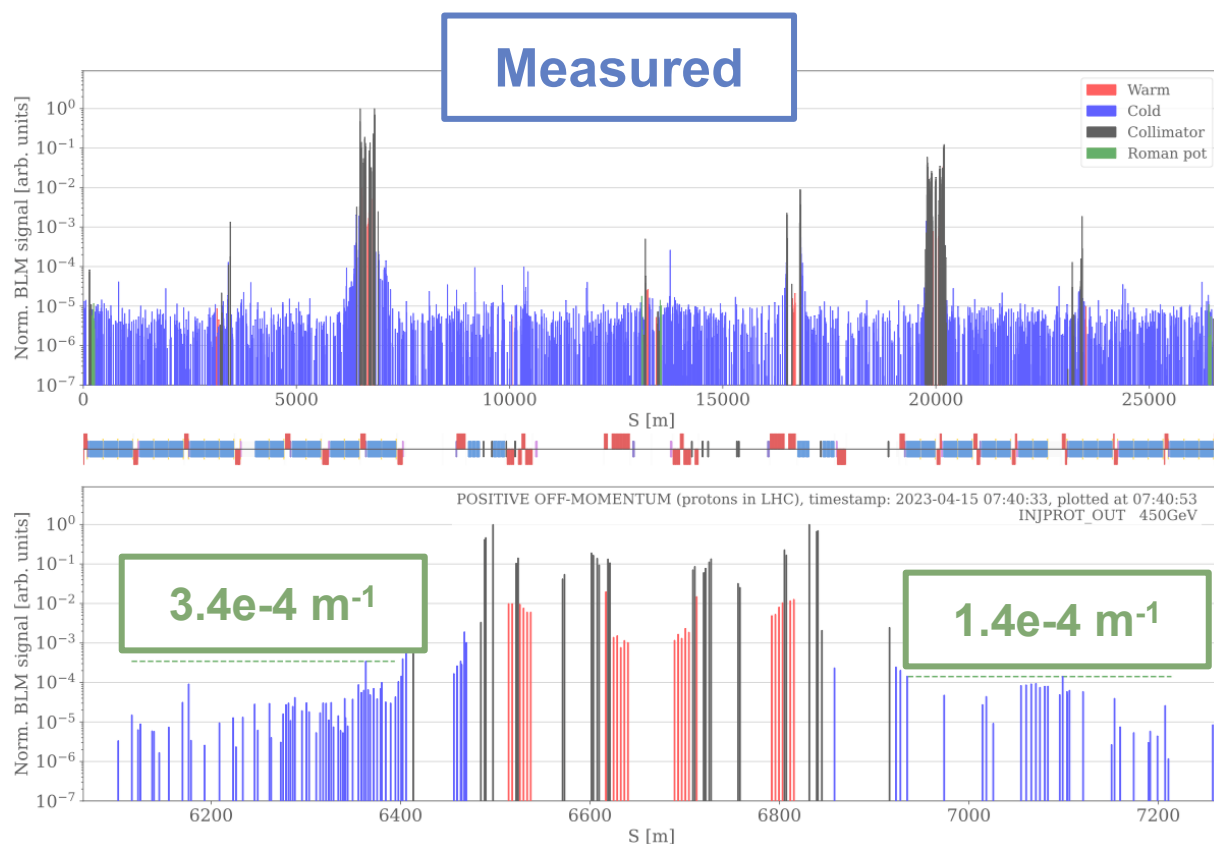


Example application:

Off-momentum cleaning

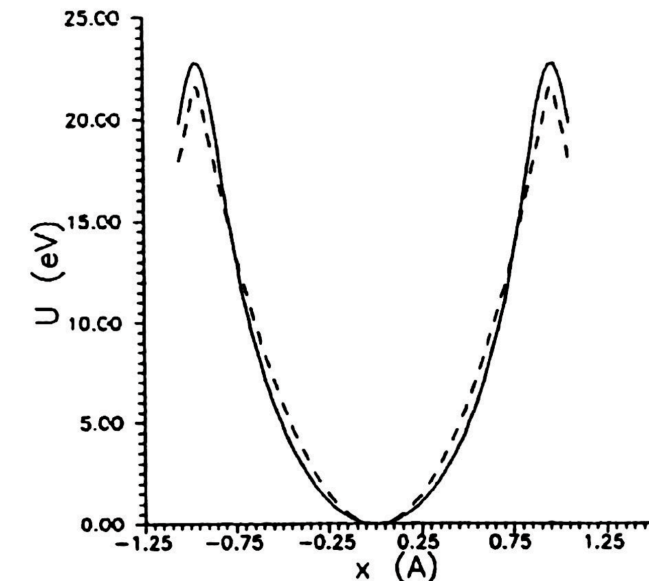
- Example **positive off-momentum** loss maps at **injection energy**, **RF sweep -200 Hz**

Off-momentum cut at
injection 3.2×10^{-3}

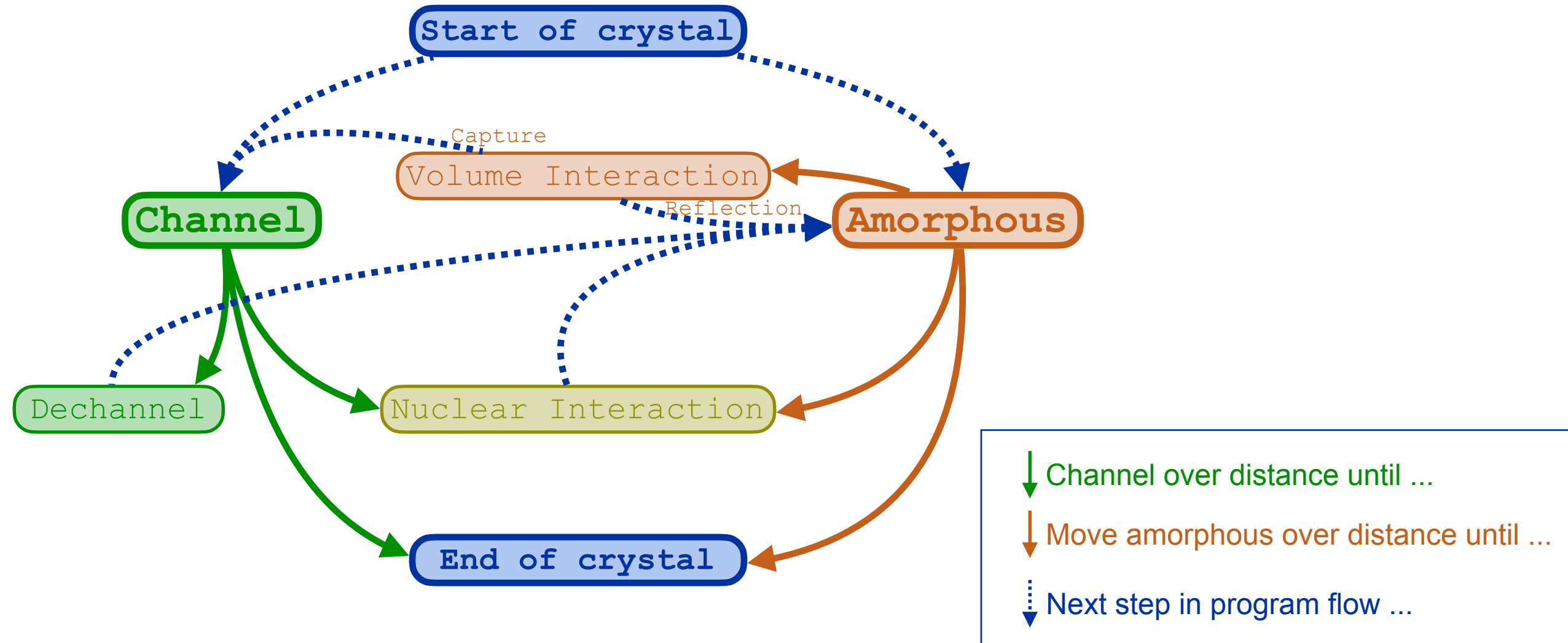


Everest Crystals

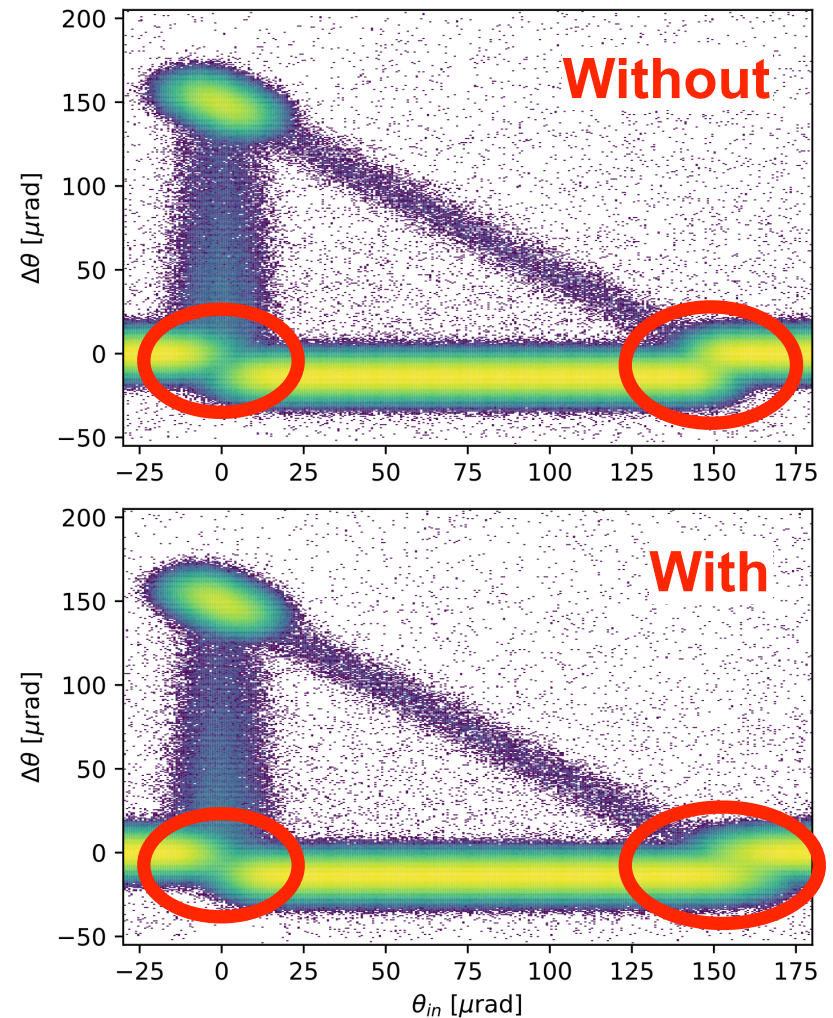
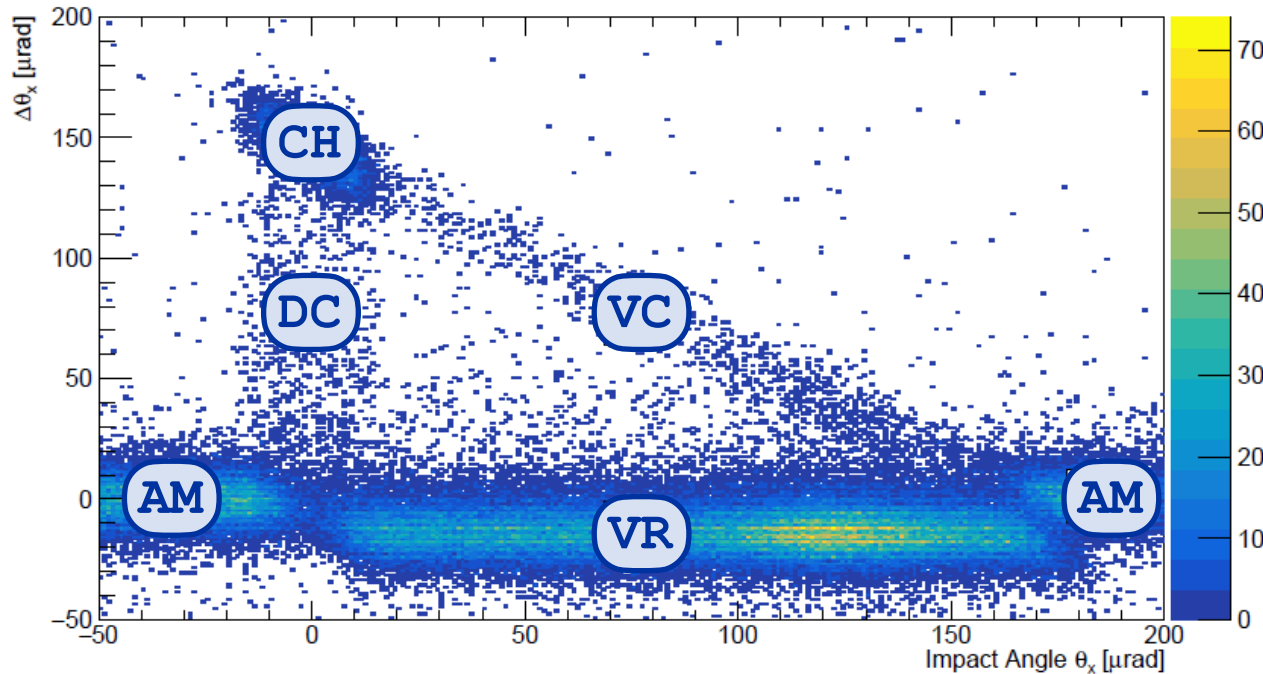
- **Complete revision** of crystal routine (both programming logic and physics)
- Needed to simulate **long crystals** (previously only single interaction possible)
- Replaced copy-pasted code with new logic
- **Low-level fixes** on physics:
 - Computation of Volume Interaction (two errors that kind of cancelled each other)
 - Bending angle was over-approximated (was still within accuracy)
 - Saturation factor of channeling probability was compensating typo
 - Hard-coded material parameters are removed
- **Work in progress:**
 - Questionable need of transition regions
 - Critical angle calculation



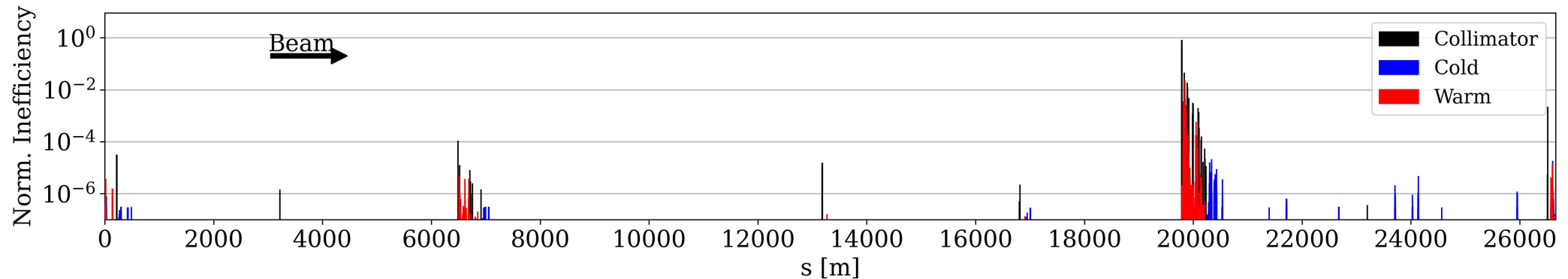
Everest Crystals: New Logic Flow



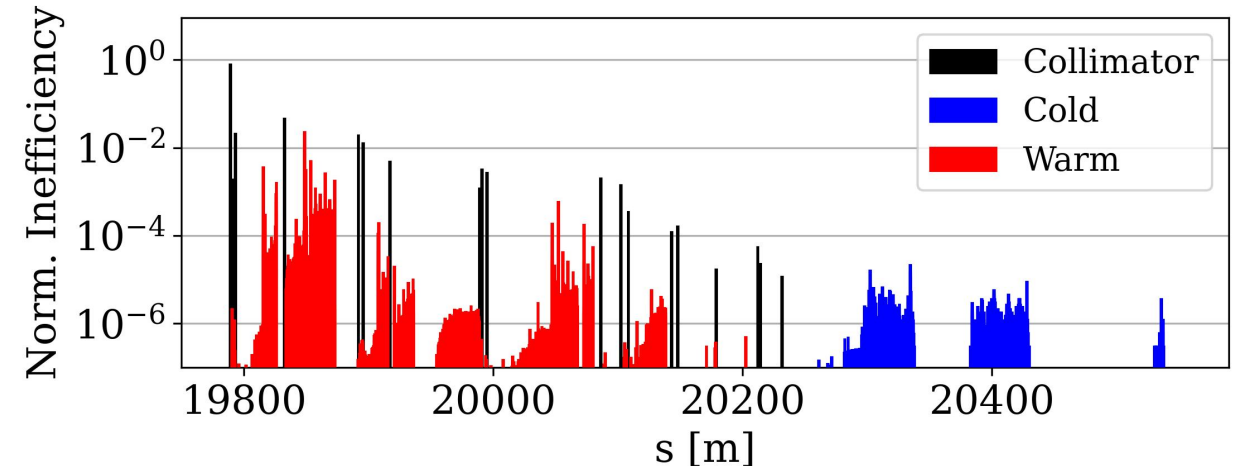
Everest Crystals: Transition Regions



- Are transition regions realistic?
- Physical motivation seems weak (geometrical constraints)
- In-depth benchmark coming up (all 3 codes + new measurements)

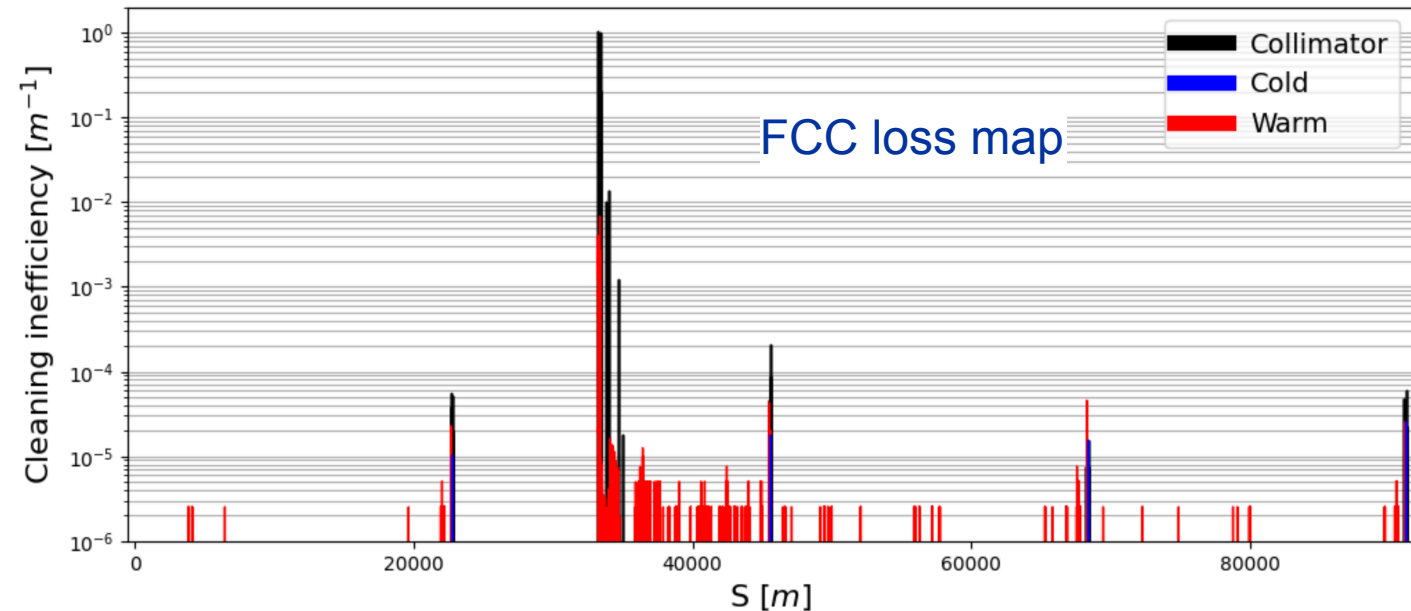


- **Large amount of progress made:** first working prototype, **fully integrated into Xcoll API!**
- Still need to manually create FLUKA input files (*.inp, using SixTrack-tuned code)
- **Everything else managed in Python:**
FLUKA, flukaserver, FlukaIO, network, ...
- Many layers:
Python => SixTrack (FORTRAN)
=> FlukaIO (FORTRAN)
=> FlukaIO (C)
=> FLUKA



- **Work in Progress:**
 - File generation based on **xt.Line** and **xc.CollimatorDatabase** in order to remove SixTrack dependency
 - Reduce programming layers: Python => xobjects C API => FlukaIO (C) => FLUKA
 - Automatic FlukaCollimator generation for standard studies
 - Retrieve more impact information (interaction type etc) from FLUKA
 - Test and benchmark time efficiency for optimal implementation

- **Working implementation of Geant4 coupling:**
BeamInteraction => collimasim => BDSIM => Geant4
- First steps made towards integration in Xcoll API (to leverage full functionality)
- Used in full production for FCC studies
- **Work in Progress:**
 - No need to use BeamInteraction
 - Reduce programming layers: Python => xobjects C API => BDSIM => Geant4



Xcoll Summary


- Very active development, several new features, more are planned
- **Quickly becoming new standard for collimation team:**
 - **Everest:** default for proton - matter interactions (K2 discontinued)
 - **Geant4:** only used with xsuite (SixTrack+Geant4 discontinued)
 - **FLUKA:** first prototype, SixTrack+FLUKA still in active use

Xcoll Summary

- **Future outlook:**
 - Detailed **manual**, including underlying physics (in progress)
 - Further remove dependency on colldb: allow easy collimator installations
 - **Everest**: detailed crystal comparison, jaw flatness models, and GPU-compatibility
 - **Geant4**: complete integration into xcoll
 - **FLUKA**: translate to C, and add user-friendly API without files


Xboinc

Facilitating large-scale volunteer computing

Development supported by  CHART

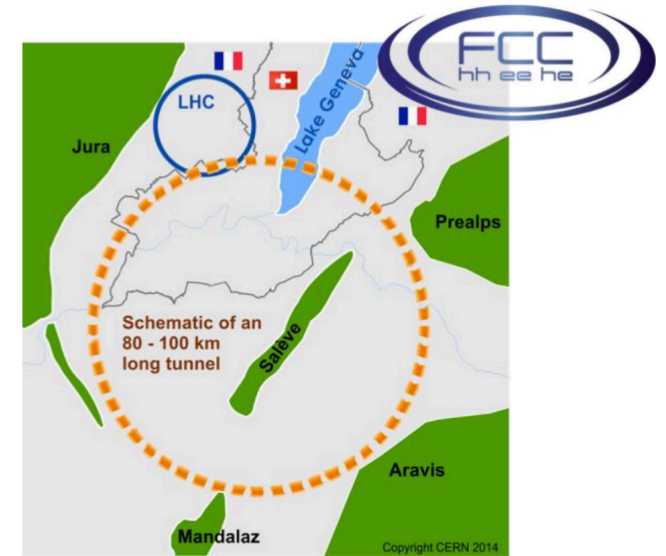
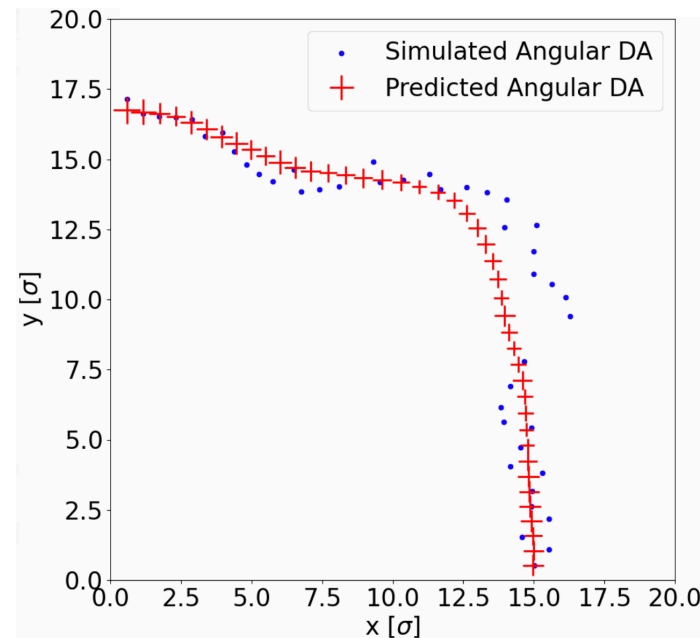
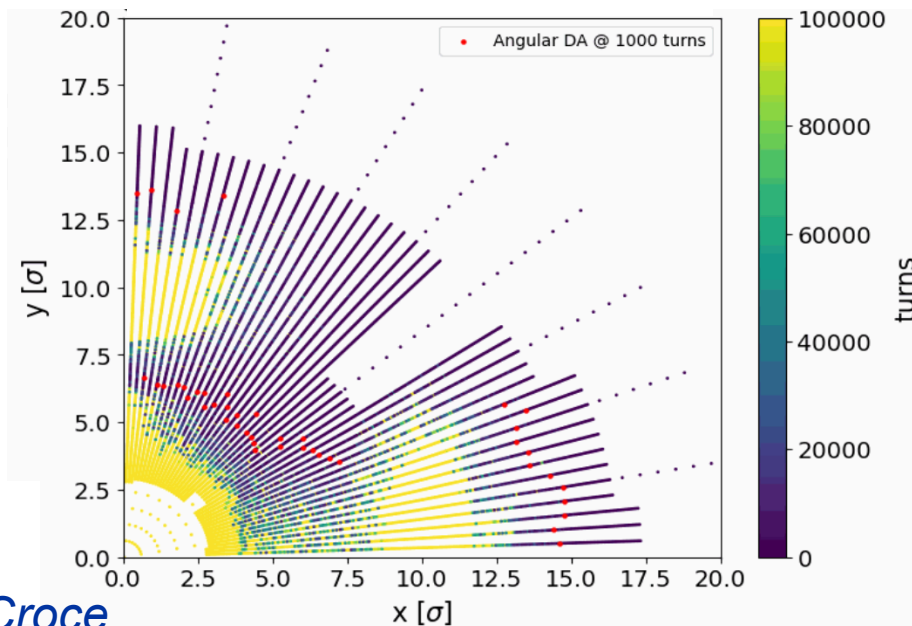
Xtrack on BOINC

- **Similar approach as SixTrack:**
 - Single light-weight application (pre-compiled stand-alone executable)
 - Custom environment (submission, assimilator, validator)
- **Current status and outlook:**
 - Executables for Windows (64 bit), Mac, and Linux on test server (lhathome-dev.cern.ch)
 - Custom server environment nearing completion
 - Not limited to one type of study (though only compileable parts of toolkit)
 - **CPU at a first stage** (investigate potential for GPUs later)

Development supported by  CHART

Xtrack on BOINC: Example study

- **Currently, most people moved to Xtrack**
(explaining the drop in SixTrack jobs submitted to BOINC)
- The tailoring of SixTrack BOINC to one type of study **limited the number of users**
- Very large-volume study in the pipeline: surrogate ML model for LHC and FCC in collaboration with EPFL, SDSC (under the CHART project)



Study supported by CHART

- To avoid compatibility issues, Xboinc version **freezes** all Xsuite packages' versions
- Generating new **executables** for CPU is now straightforward (with collimation included)
- Logic flow:
 - User registration on server ✓
 - User submits jobs using xboinc.SubmitJobs ✓ (on user EOS or AFS workspace)
 - Xboinc-server fetches jobs from user workspace ✓
 - Xboinc-server submits to BOINC ✓
 - Xboinc-server retrieves results ✓ and organises them by user and type **WIP**
 - User reads results using xboinc.retrieve **WIP**
- Careful development (thorough testing and documenting) of Xboinc-server because of **scalability**

Xboinc Outlook

- **Current users (SixTrack):** ~1 (will move to xboinc soon)
- **In development:**
 - Finish automatic retrieval and return of jobs
 - Address credit issue by smart sampling of initial conditions
 - Add encoding to protect against cheaters (currently only in conceptual phase)
- **We need users!** (not enough jobs - volunteers are eager to crunch)
 - Not only DA studies, but any non-collective (compilable to C) study

Xdyna

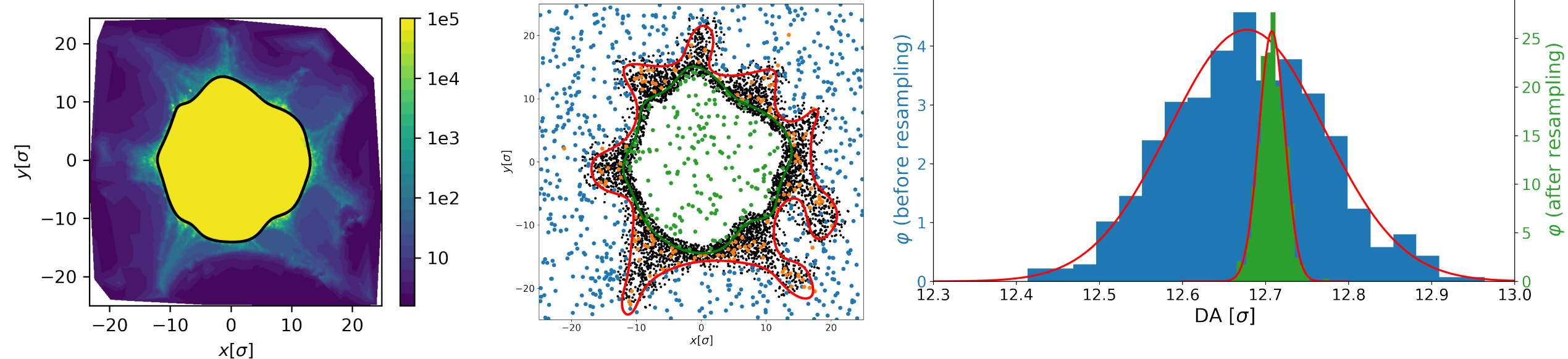
Dynamic aperture is fun

- Xdyna is the **Xsuite successor of SixDesk**, expanding its functionality
- Initial conditions can be radial, on a grid, or random (with resampling)
- In active development, with several new DA border detection methods ("classical" and ML)
- An improved **fitting algorithm** to describe the **evolution of DA** is work in progress
- A lot of progress, on using **dynamic indicators** to describe chaos, is being merged

- **Small team of users, feel free to join**

ML Border Detection

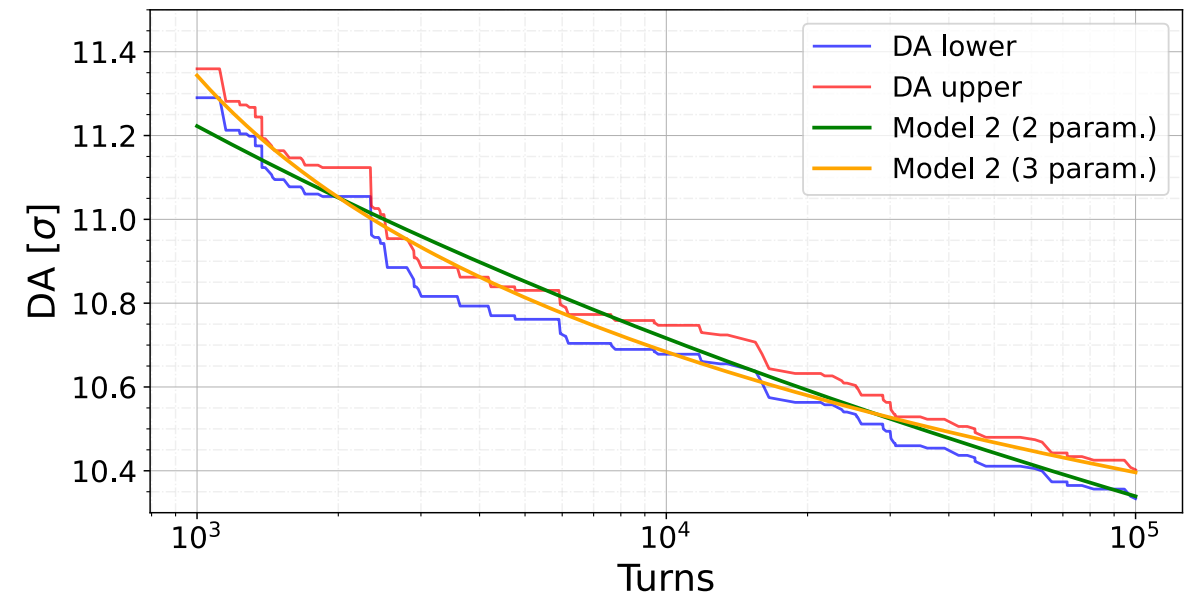
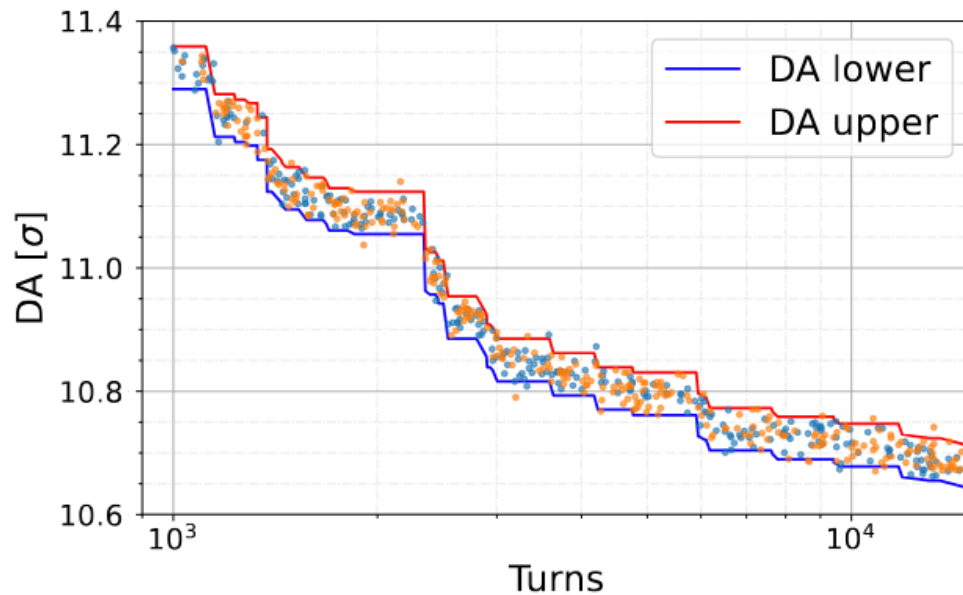
- The border of stability in phase space exhibits chaotic behaviour
- High resolution is desirable for more accurate evolution (and hence extrapolation) but not known in advance where to sample more initial conditions
- Xdyna provides ML Border models to iteratively recognise the region of stable particles



Describing the evolution of DA

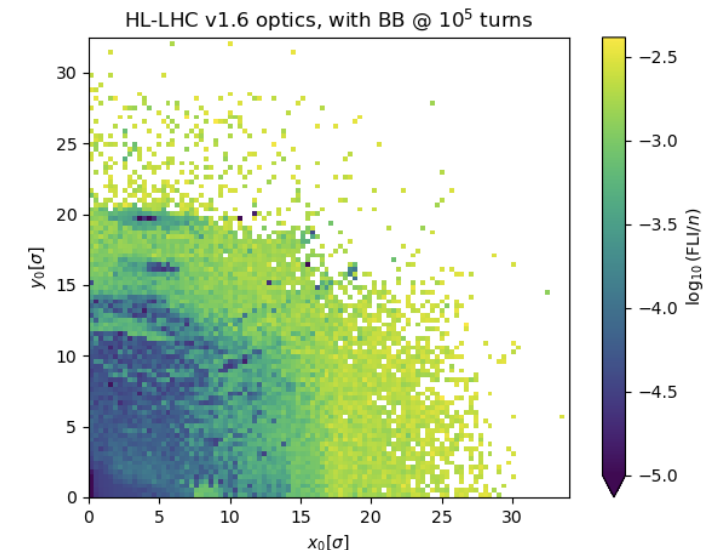
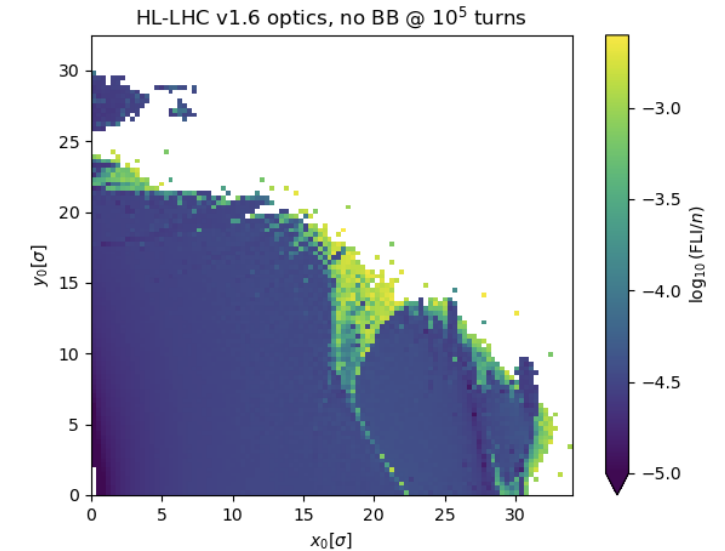
T. Pognat, FFVdV

- 2 DA estimations: **lower** (last surviving) and **upper** (first loss) (SixDesk used lower)
- Implementation of DA evolution with recent models, use sampling to improve fitting
- Exploring different fitting methods, tuning of border detection, order of integrator, sampling distribution, ...



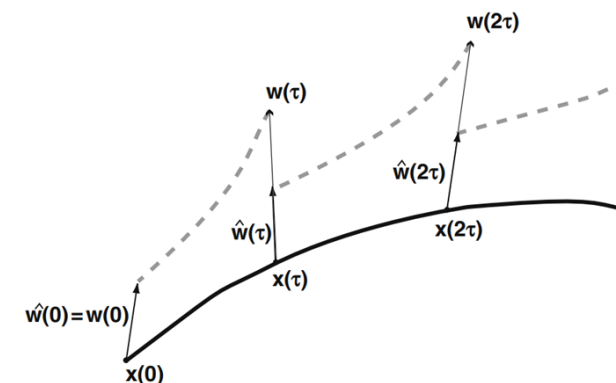
Chaos indicators (pre-alpha)

- Mathematical tools to inspect **chaoticity** of the phase-space
- Well established tools such as **Fast Lyapunov Indicators (FLI)** and **Frequency Map Analysis (FMA)**, and more novel tools
 - Recently investigated [here](#)
- More details **today** at [NLBD-WG](#)
- Need proper testing, and finish implementation into Xdyna
- Pre-alpha stage on [GitHub fork](#)



Tools for evaluating FLI

- Use **ghost particle** method to evaluate FLI:
 - for each particle, track a displaced particle and evaluate the evolving distance turn by turn
 - necessary to renormalize the distance while also keeping track of the accumulated distance
- The **GhostParticleManager** object offers the possibility to track multiple ghost particles with ease:
 - can be executed on CupyContext without breaking parallelism
 - supports displacements and renormalisations in normalised coordinates (good for avoiding geometrical biases!)



```
# create the ghost particles
manager = GhostParticleManager(
    particles,
    context,
    use_norm_coord=True if "norm" in yaml_dict["displacement_method"] else False,
    twiss=twiss,
    nemitt_x=2.5e-6,
    nemitt_y=2.5e-6,
    nemitt_z=EW_GIVEN if yaml_dict["displacement_method"] == "norm_z" else None,
)

if "norm" in yaml_dict["displacement_method"]:
    manager.add_displacement(
        module=yaml_dict["displacement_module"], direction="x_norm"
    )
    manager.add_displacement(
        module=yaml_dict["displacement_module"], direction="px_norm"
    )
    manager.add_displacement(
        module=yaml_dict["displacement_module"], direction="y_norm"
    )
```

```
track_displacement(
    manager,
    line,
    yaml_dict["sampling_turns"],
    outfile,
    yaml_dict["realign_frequency"],
)
```


Conclusions

Cool stuff, right?

Thanks for your attention!

Feel free to use at will, comment/correct/contribute!





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