Towards a Model Driven Accelerator with Peta-scale Computing

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Outline

- **What & Why ?** **Concept & Motivations for the Model Driven Accelerator**
- **What we need ?** **Requirements to Realize the Model Driven Accelerator**
- **What we have done ?** **Developments along three major axes**
  - **- Realistic 3D Beam Dynamics Code**
  - **- Appropriate Optimization Tools (Applicable to real machines)**
  - **- Large Scale Parallel Computing**
- **What we need to do ?** **Further Developments**
  - **- A lot …**
- **Summary**

Model Driven Accelerator: Concept & Motivations

- **The Concept:** Use a computer model to fully support real-time accelerator operations.

- **Present Situation:** No accelerator in the world can fully rely on a computer model for its operations.

- **Possible Reasons:** Discontinuity between the design and operations phases
  - Design and simulations assume almost perfect conditions.
  - Elements specs are usually different from their original design.
  - Not enough diagnostics to characterize the machine.

- **Consequences:** Delay in commissioning and low machine availability.
  - Simulations cannot reproduce the measured data.
  - A lot of work to deliver the first beam during commissioning.
  - A lot of time spent on beam tuning/retuning during operations.

Model Driven Accelerator: Concept & Motivations

- **For Example:** RIA / FRIB Cannot afford “manual” operations …
  - Primary beams: p to U, from 200 MeV/u to 600 MeV/u
  - Secondary beams: all over the map …

➢ **Need a realistic computer model for the machine to support commissioning and operations**

- **The Benefits:**
  - Fast tuning for the desired beam conditions.
  - Fast retuning to restore the beam after a failure.
  - Increase the availability of the machine.
  - Reduce the operating budget.

- **The Means:**
  - A realistic 3D model of the actual machine.
  - Fast turn-around optimizations to support decision making.

Realization of the Model Driven Accelerator: What we need ?

- **Need a realistic 3D beam dynamics code with the appropriate set of optimization tools and large scale parallel computing capability.**

- **Why a beam dynamics code ?**
  - More realistic: 3D fields including fringe fields and SC calculations
  - More detailed: Beam halo, beam loss, …
  - Produce detector-like data: Profiles, distributions, …

- **Why more optimization tools ?**
  - Optimization tools are needed not only in the design phase but also to tailor the model to the actual machine to be used for real-time operations.

- **Why large scale computing ?**
  - Optimizations of large number of parameters with a large number of particles for large number of iterations require large scale computing.

- **The beam dynamics code TRACK is being developed at Argonne to meet these requirements.**

1- A Realistic Beam Dynamics Code

The Beam Dynamics Code: TRACK

➢ TRACK Main Features

- A wide range of E-M elements with 3D fields
- End-to-end simulations from source to target
- Simultaneous tracking of Multiple charge states heavy ion beams
- Interaction of heavy ion beams with strippers
- Automatic transverse and longitudinal beam tuning
- Error simulations for all elements: Static and dynamic errors
- Realistic correction procedure: Transverse and Longitudinal
- Simulations with large number of particles for large number of seeds
- Beam loss analysis with exact location of particle loss

➢ Recent Updates

- Possibility of fitting experimental data: beam profiles, …
- H- Stripping: Black body, Residual gas and Lorentz stripping
- The design and simulation of electron linacs
- Parallel version is fully developed with good scaling up to 32K processors
- Possibility of simulating the actual number of particles in a bunch

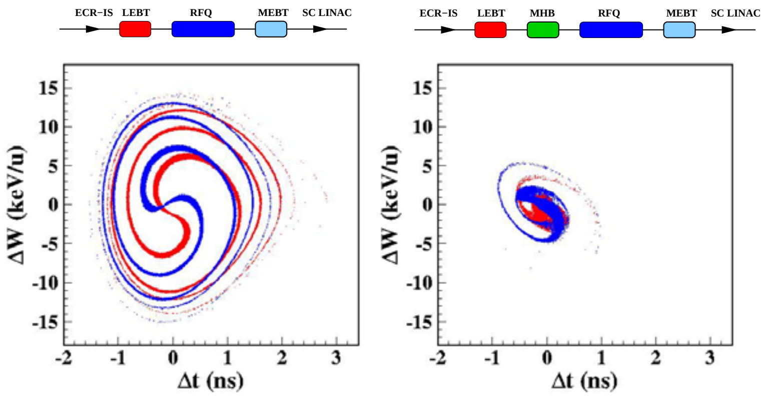
TRACK: Extensive List of Supported Elements

- Any type of RF resonator (3D fields)
- Static ion optics devices (3D fields)
- Radio-Frequency Quadrupoles (RFQ)
- Drift Tube Linacs (DTL)
- Coupled Cavity Linacs (CCL)
- Solenoids with fringe fields (model and 3D fields)
- Bending magnets with fringe fields (model and 3D fields)
- Electrostatic and magnetic multipoles
- Multi- Harmonic Bunchers (MHB)
- Axial Symmetric electrostatic lenses
- Entrance and exit of HV decks
- Accelerating tubes with DC voltage
- Transverse beam steering elements
- Stripping foils or films for heavy-ion beams
- Horizontal and vertical jaw slits

➢ **TRACK was heavily used in the design and simulations of the RIA/FRIB and FNAL-PD linacs and recently in the simulation of the SNS linac.**

TRACK Application: Design and Simulations of the FRIB Linac

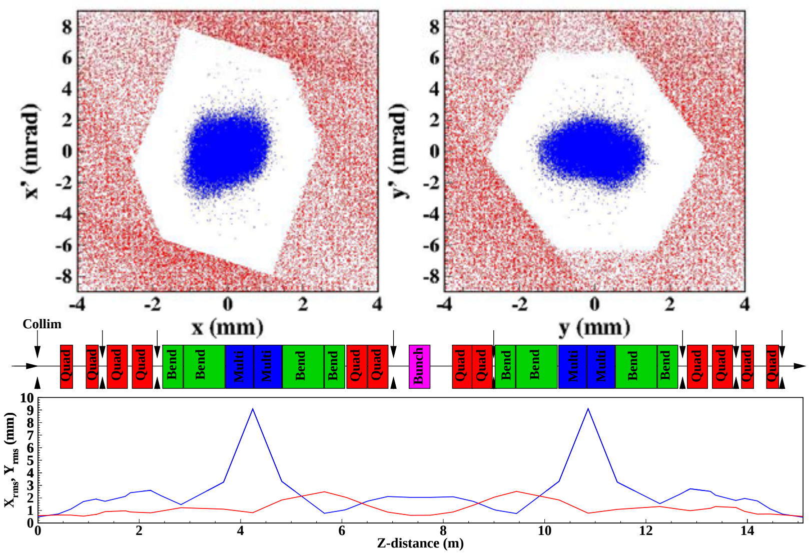
Injector: Two options w/wo MHB



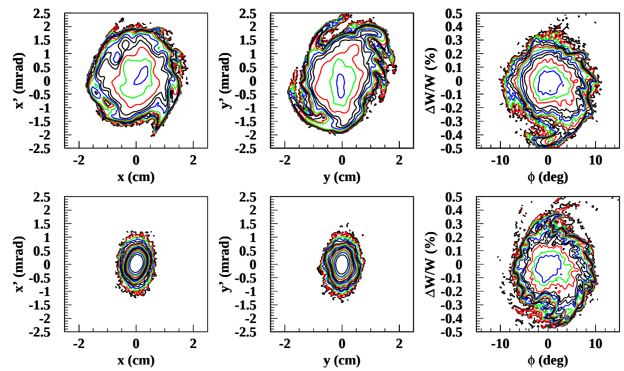
100 % Transmission
Large long. emittance

80% Transmission
~ 8 times smaller emittance

Chicane: Collimation and Matching



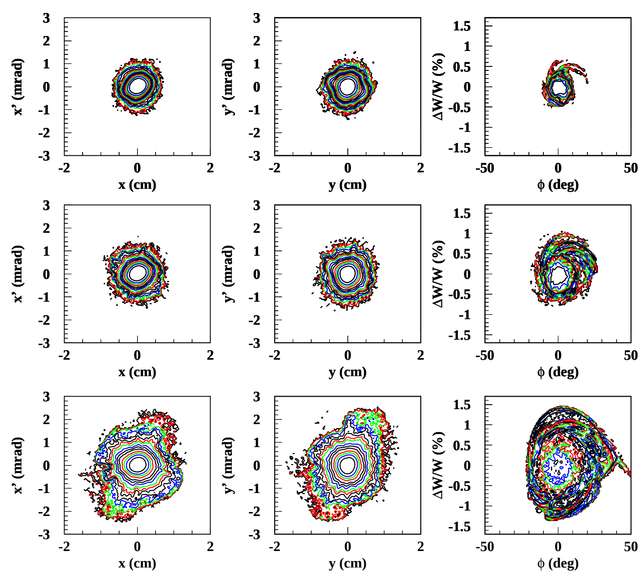
Error simulations: Before and after Corrections



No corrections

Corrections

Different RF jitter errors: 0.5, 1 and 2 (deg, %)



0.5 deg, 0.5 %

1.0 deg, 1.0 %

2.0 deg, 2.0 %

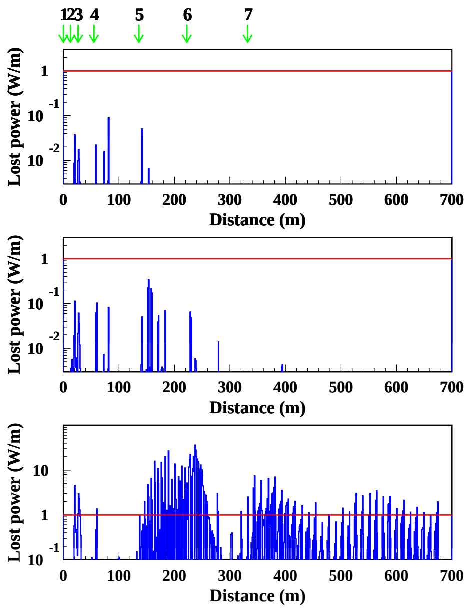
TRACK Application: Design and Simulations of the FNAL-PD

Error simulations: 100 seeds, 1M particles each

Table: Errors and their typical values

Error	Value	Distr.
Cav. end displacement		Uniform
RT and SC spoke cav.	0.5 mm (max)	
SC elliptical cav.	1.0 mm (max)	
Sol. end displacement		Uniform
Type 1 (18 cm long)	0.15mm (max)	
Type 1 (32 cm long)	0.2 mm (max)	
Quad. end displacement	0.15mm (max)	Uniform
Quad. rotation (z-axis)	5 mrad (max)	Uniform
Cav. field jitter error	0.5 % (rms)	Gaussian
Cav. phase jitter error	0.5°(rms)	Gaussian

Beam Loss: Different RF errors



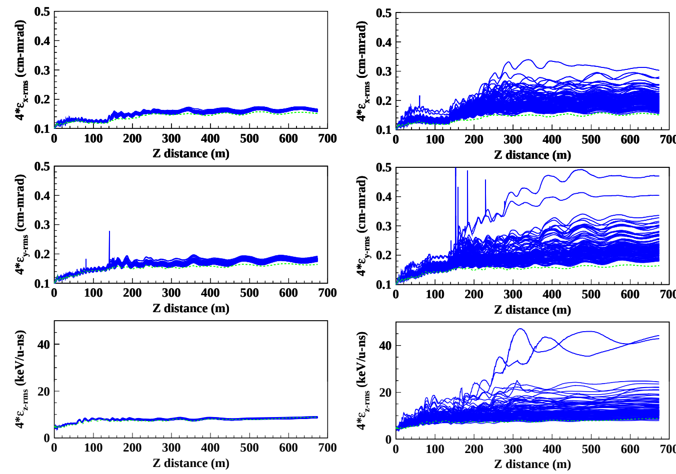
0 deg
0 % — Fraction: 2E-5
Peak: 0.1 W/m

1 deg
1 % — Fraction: 1E-4
Peak: 0.4 W/m

2 deg
2 % — Fraction: 3E-2
Peak: 35 W/m

Beam Emittances: before and after RF errors

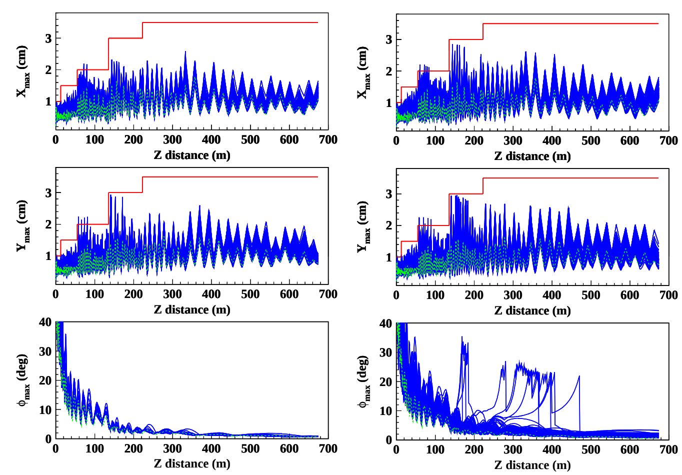
0 deg
0 %



1 deg
1 %

Beam Envelopes

0 deg
0 %



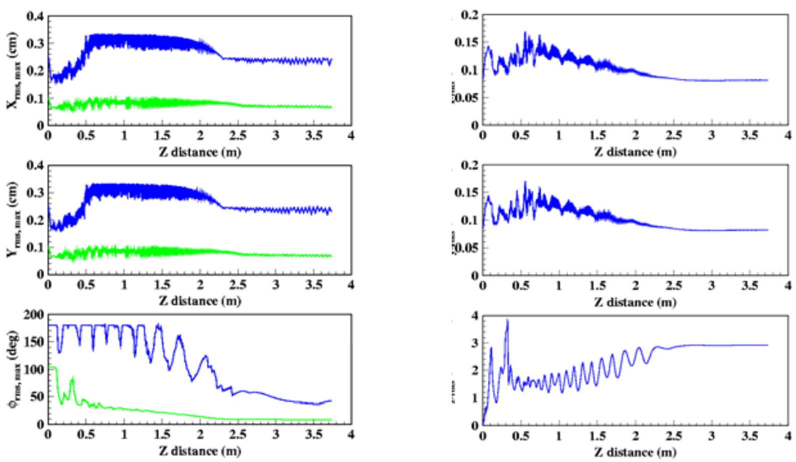
1 deg
1 %

➢ See Paper TH301, P. Ostroumov et al.

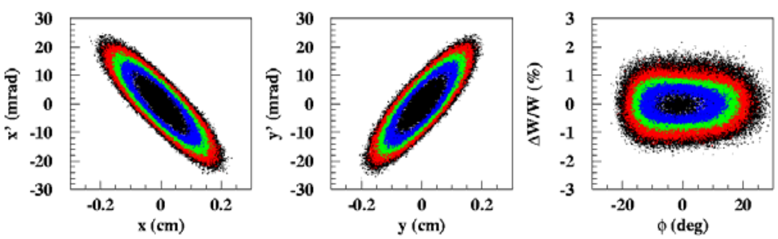
TRACK Application: End-to-end Simulation of the SNS Linac

RFQ Simulations

Envelopes: rms, max | **Emittances: 4*rms**



Phase space plots

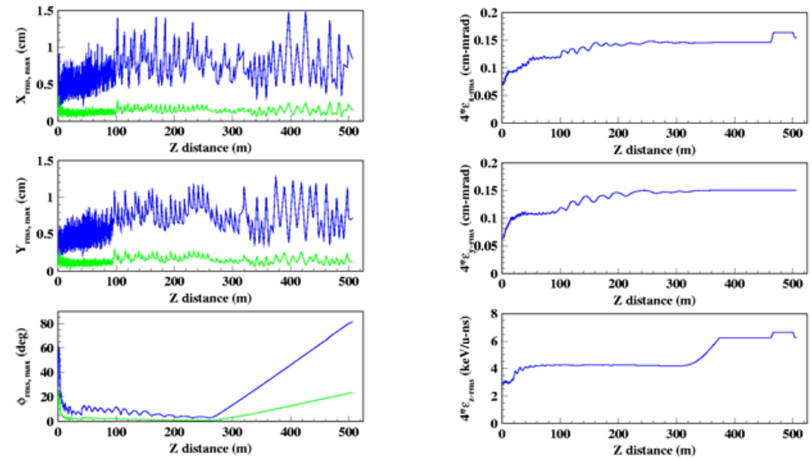


Transmission

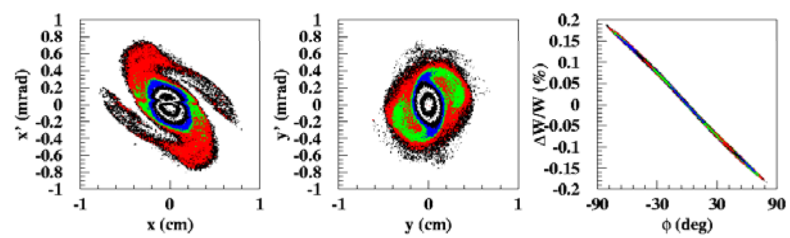
Current	Parmteq	TRACK
0 mA	99.4 %	98.5 %
32 mA	97.3 %	91.4 %
60 mA	90.0 %	70.0 %

Linac simulations from MEBT to HEBT

Envelopes: rms, max | **Emittances: 4*rms**



Phase space plots

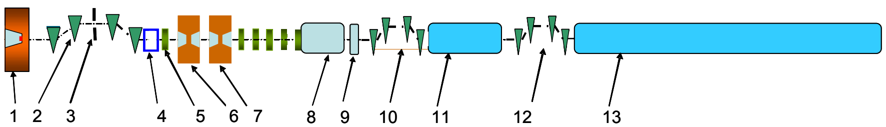


- **See Paper MOP091, B. Mustapha et al.**

- **Next steps**
  - Error and beam loss simulations
  - Compare with experimental data

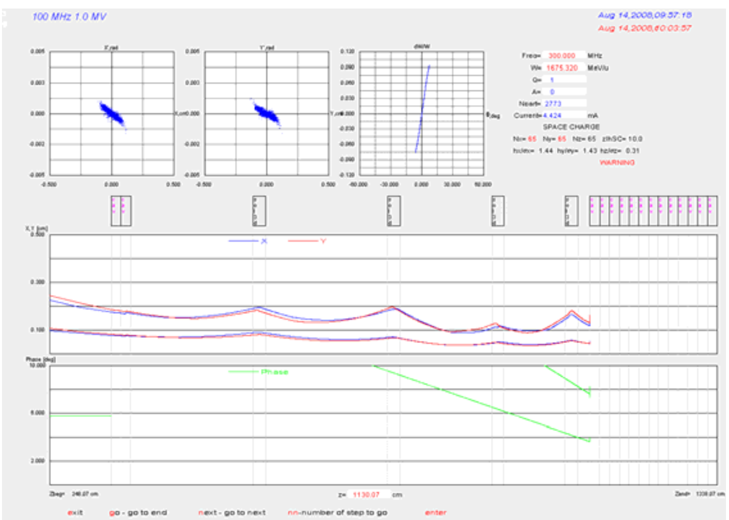
TRACK Application: Design and Simulations of an electron linac

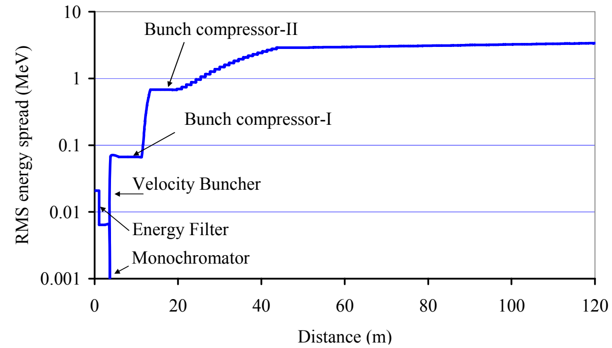
Layout of a linac for a future X-Ray FEL Oscillator



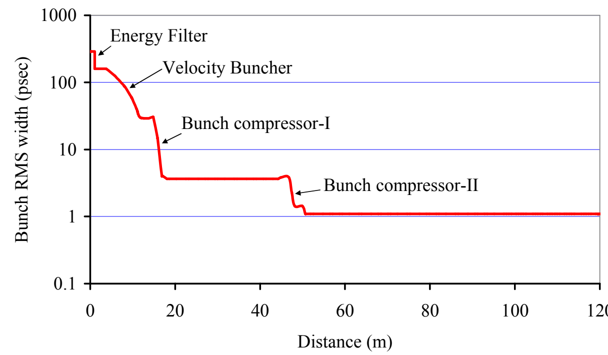
1- RF cavity with thermionic cathode, 100 MHz, 1 MV; 2- chicane and slits; 3- as an energy filter; 4- quadrupole triplet; 5- focusing solenoid; 6- monochromator of the beam energy, f=600 MHz; 7- buncher, f=300 MHz; 8- booster linac section, f=400 MHz; 9- RF cosine-chopper to form rep. rate 1 MHz to 100 MHz; 10- bunch compressor – I; 11- SC linac section, 460 MeV, f=1300 MHz; 12- bunch compressor – II; 13- initial section of the SC linac, f=1300 MHz.

Beam Simulations

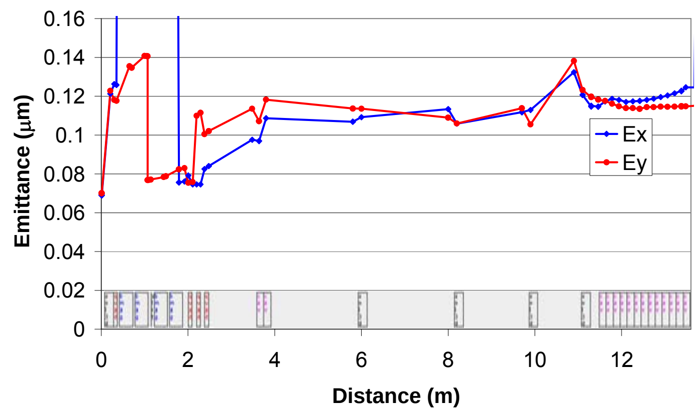




Energy spread



Bunch width



Emittance

➢ **See Paper TUP117, P. Ostroumov et al.**

2- Appropriate Optimization Tools

Optimization Tools: Different tools for different phases

- An accelerator project may be sub-divided into three phases, namely the design, commissioning and operations phases. The optimization needs are different for the different phases.

- **Design:** Optimize the design parameters for different design options to produce a robust and cost-effective design → Fit for the best general beam properties

- **Commissioning:** Tailor the computer model to the actual machine by reproducing the experimental data at beam diagnostic points → Fit the data

- **Operations:** Use the computer model to retune the machine or to rapidly restore the beam after a failure with limited beam loss → Fit element settings for desired beam conditions

> **The computer model needs to be tailored to the actual machine during commissioning to be used for real-time operations.**

Example of Optimization Tools Developed for TRACK

- Automatic transverse and longitudinal tuning of a multiple charge state heavy ion beam in a given linac section by varying focusing field strengths, RF phases and amplitues: ~ 100 or more parameters.

- Automatic longitudinal fine tuning to reduce the longitudinal emittance of a multiple charge state beam before a stripper to reduce beam loss in the following section.

- Realistic corrective steering based on beam center measurements.

- Fit experimentally measured beam profiles to extract the beam parameters (emittances and Twiss parameters) at a given point to use for further simulations.

- Find element settings in an achromatic transport system to produce symmetric beam dynamics.

➢ **More optimization tools are under development …**

Automatic Transverse Tuning: Application to RIA/FRIB Linac

- **Purpose:** Tune the linac for a given beam and produce smooth transverse beam dynamics.

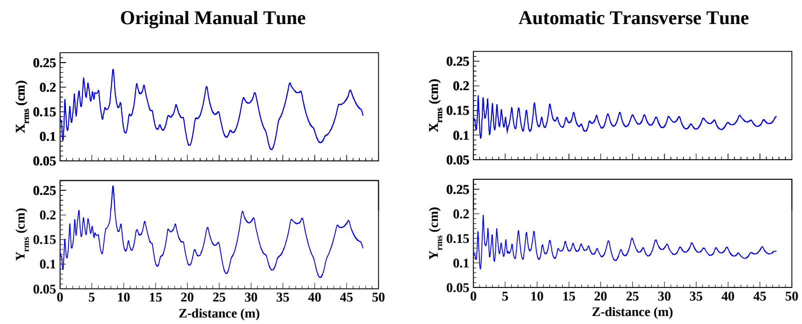
- **Method:** Minimize the fluctuations in the RMS beam sizes along the considered section.

- **Fit Function:** $F = X^0_{rms} + \sum_i \frac{(X^i_{rms} - X^0_{rms})^2}{\varepsilon^2_{X_{rms}}} + Y^0_{rms} + \sum_i \frac{(Y^i_{rms} - Y^0_{rms})^2}{\varepsilon^2_{Y_{rms}}}$

  where X^0_{rms} and Y^0_{rms} are the RMS beam sizes at the entrance of the section or after the first focusing period, the sum index i runs over the focusing periods in a given section and ε_{Xrms} and ε_{Yrms} are the allowed errors on the RMS beam sizes.

- **Fit Parameters:** Field strengths in focusing elements

- **This method is general and should produce good results for both periodic or non periodic accelerating structures.**



X- and Y-rms beam sizes before and after applying the automatic transverse tuning procedure.
The beam is a two-charge state uranium beam in the first section of the RIA/FRIB driver linac.

✓ **A similar procedure was developed to produce smooth longitudinal envelopes by fitting the RF cavities field amplitudes and phases.**

➢ **Developed and used for design optimization this procedure could very well be applied to a real machine using beam profile measurements to reduce beam mismatch.**

Longitudinal fine tuning: Minimize Emittance at the Stripper

- **Purpose:** Tune a linac section to minimize the logitudinal emittance of a multiple charge state beam right before stripping.

- **Method:** Match the longitudinal beam centers and Twiss parameters of the different charge state beams:

$$W_{q0} \rightarrow W_0;\ \Delta W_{qi} \rightarrow 0; \Delta \phi_{qi} \rightarrow 0; \alpha_{qi} \rightarrow 0; \beta_{qi} \rightarrow \min$$

- **Fit Function:**

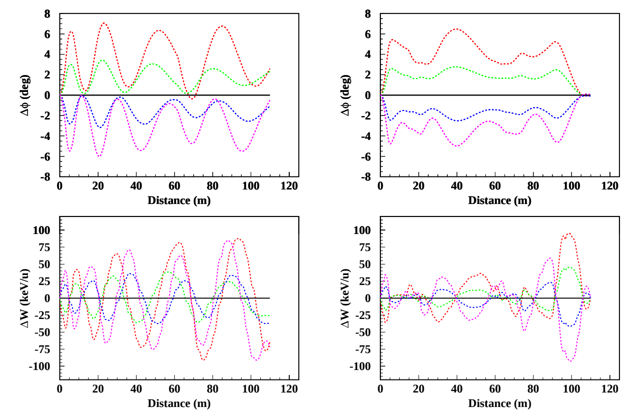
$$F = \frac{(W_{q0} - W_0)^2}{\varepsilon_w^2} + \sum_{qi} \frac{\Delta W_{qi}^{\ 2}}{\varepsilon_{\Delta w}^2} + \sum_{qi} \frac{\Delta \phi_{qi}^{\ 2}}{\varepsilon_{\Delta \phi}^2} + \sum_{qi} \frac{\alpha_{qi}^{\ 2}}{\varepsilon_{\alpha}^2} + \sum_{qi} \beta_{qi}$$

where W_0 is the desired beam energy and ε_W is the corresponding error.

$\varepsilon_{\Delta W}, \varepsilon_{\Delta \phi}, \varepsilon_{\alpha}$ are the allowed errors on the relative energy, phase and α shifts of the individual charge state beams from the central beam.

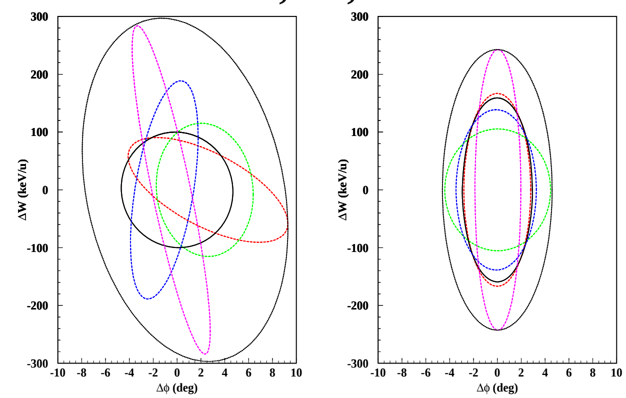
- **Fit Parameters:** RF cavities field amplitudes and phases.

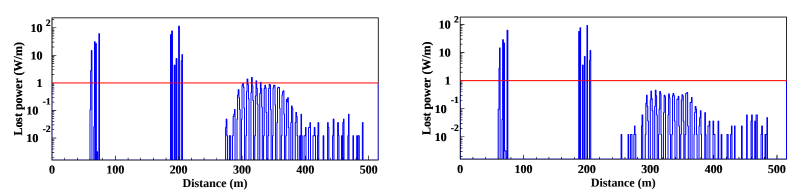
➢ **Measuring the energy and phase of individual charge states, we should be able to match their beam centers, …**



Black: Ref. 74+ of U-238

Colors: 72+,73+,75+ and 76+

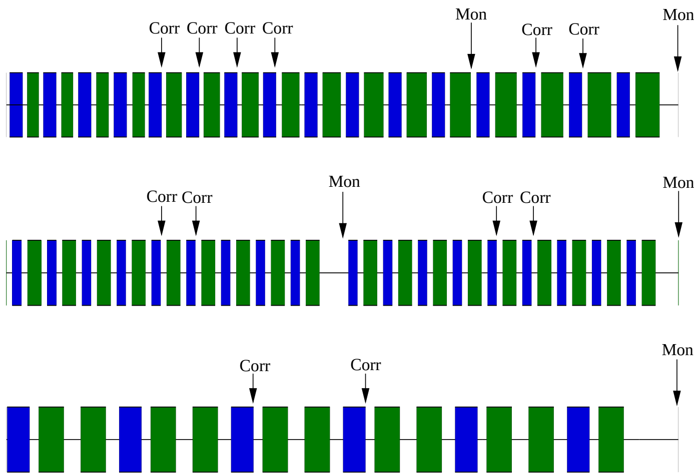


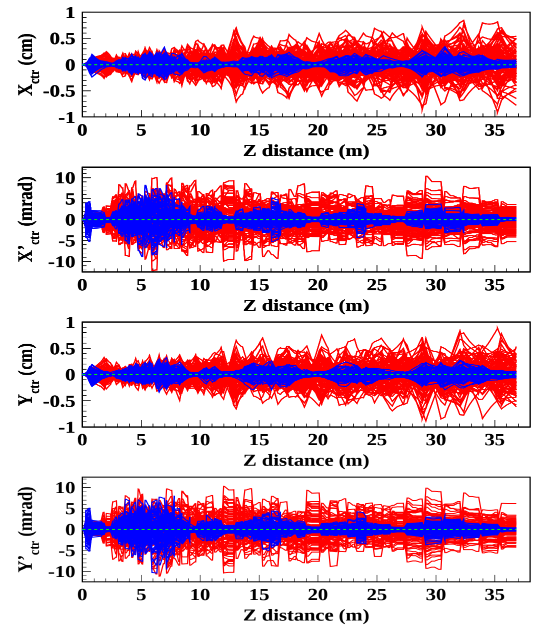


Reduced beam loss in the high-energy section

Realistic Corrective Steering: Front-end of FNAL-PD

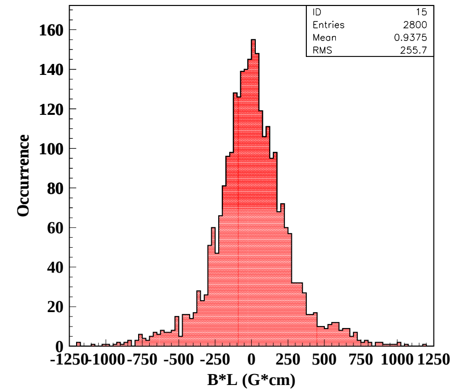
Virtual monitors and correctors are used





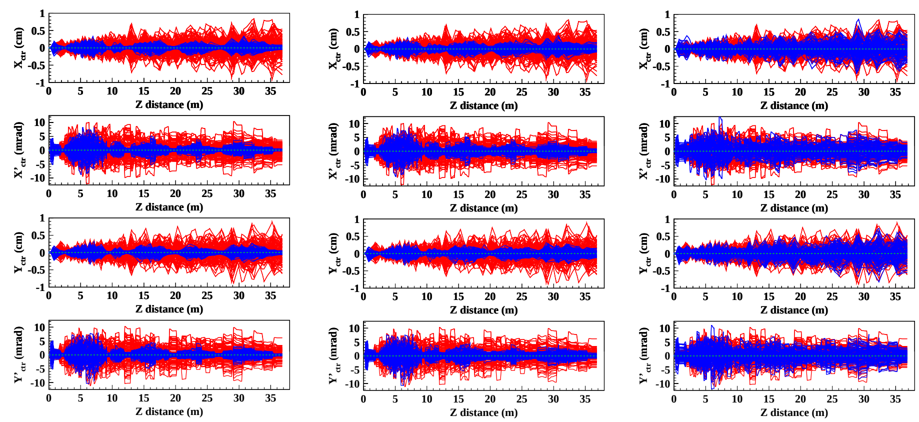
← Beam centers and angles before and after corrections

Correctors field strengths



The number and locations of monitors and correctors are varied until a reasonable correction scheme is obtained.

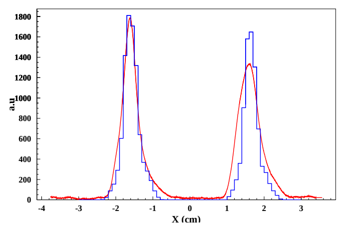
Sensitivity to monitors errors: 10, 30 and 100 μ

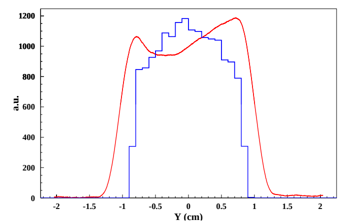


- ➢Design: the procedure was used to optimize the number, location of monitors and correctors as well as the correctors strengths.
- ➢Operations: could be easily implemented using real beam position monitors and beam steerers.

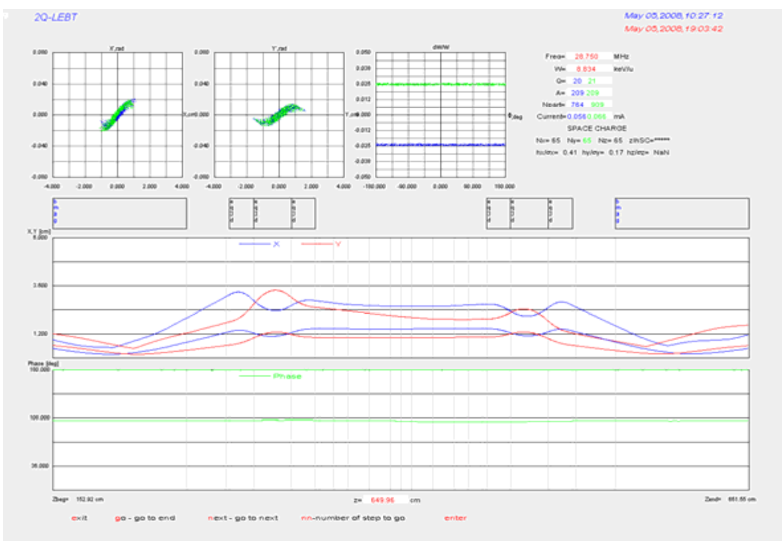
Operations of a Multi-Q Injector: Fit Data & Find Settings

TRACK fit of measured profiles to extract the initial beam parameters at the source.

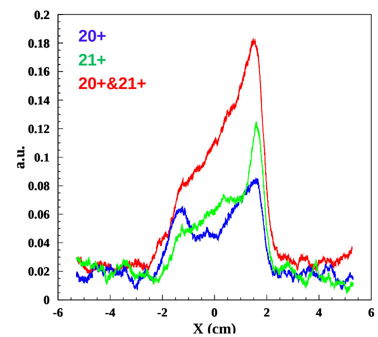


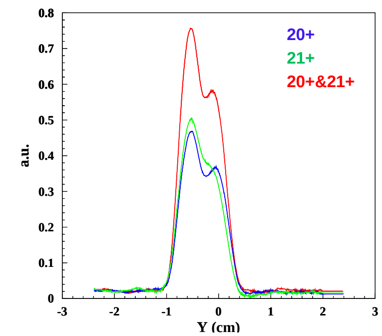


TRACK fit to find the quads setting to recombine the two charge state Bi-209 beams at the end of the LEBT.

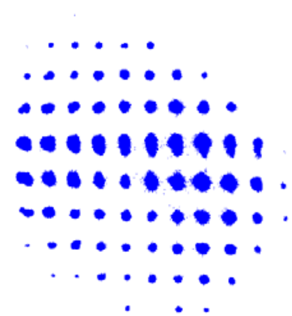


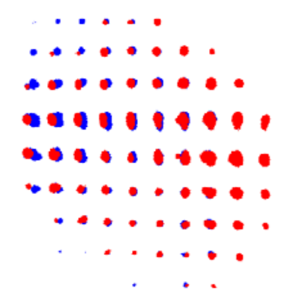
Measured beam profiles at the end of LEBT: left: horizontal, right: vertical.





Pepper-Pot images: Bi-209 beams
left: 20+&21+
right: 20+: blue, 21+:red.



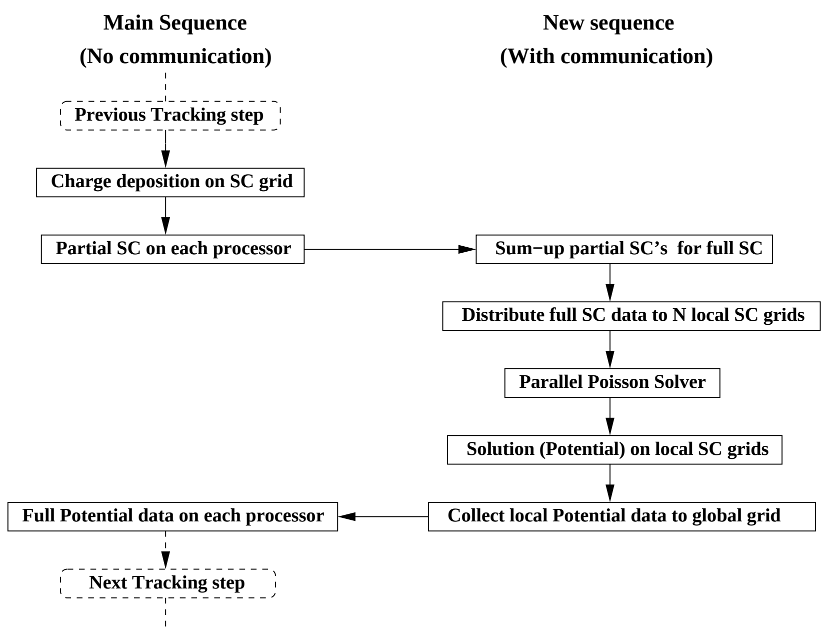


- **Such a perfect recombination was not possible without a realistic simulation.**
- **See Paper TUP118, P. Ostroumov et al.**

3- Large Scale Parallel Computing

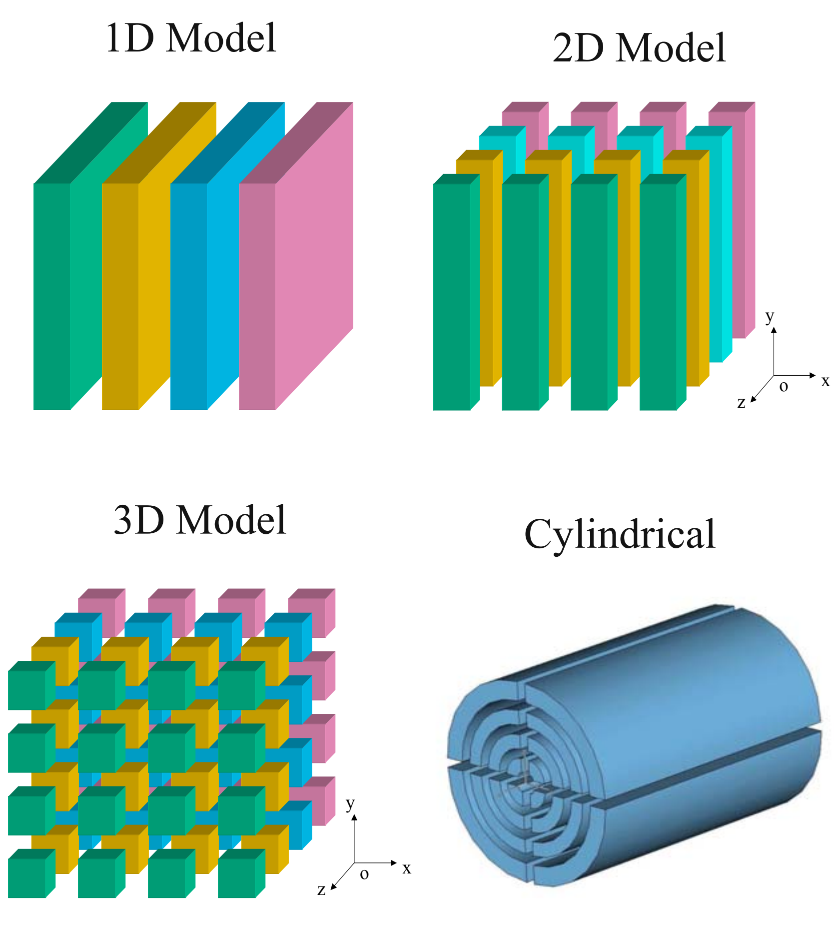
The Parallel Beam Dynamics Code: P-TRACK

Parallel Algorithm



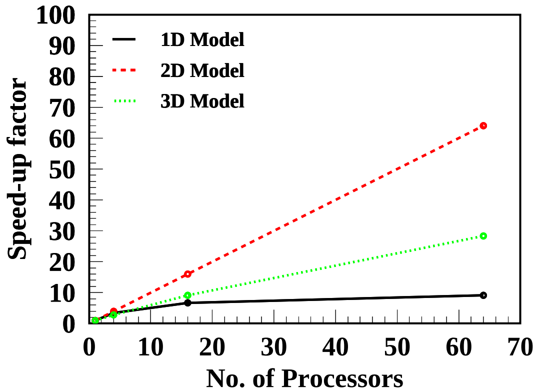
- No load balance issues once the particles are equitably shared among processors
- Very good scaling expected for very large number of particles.
- Full external field table and SC grid on every processor: possible memory limitation on some systems.

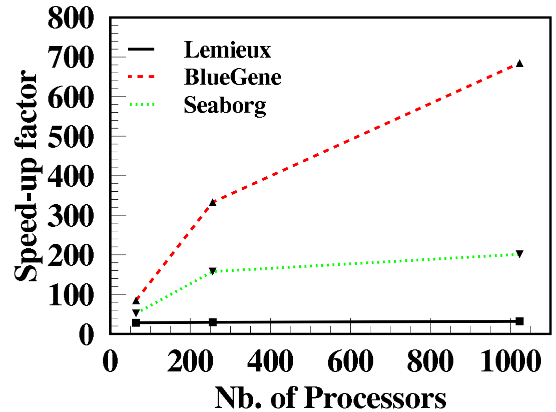
Parallel Models for Poisson's Equation



Scaling of P-TRACK with large number of processors

- TRACK scaling with number of processors on different platforms.





- TRACK weak and strong scaling on the Blue-Gene machine at Argonne

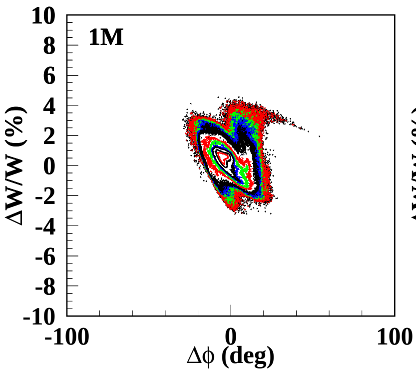
CPU	Time/cell (s)	Particle #	Parallel Efficiency
256	384	55M	100%
512	384	110M	100%
1024	388.7	220M	98.8%
2048	400.6	440M	95.8%
4096	385	880M	99%

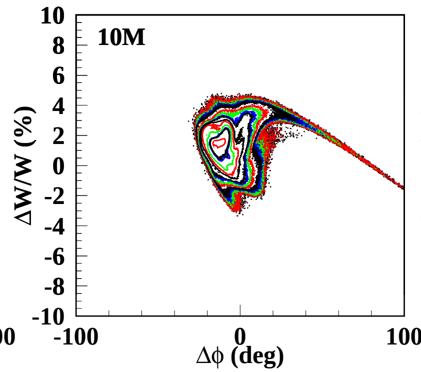
Strong scaling for 110 M particles

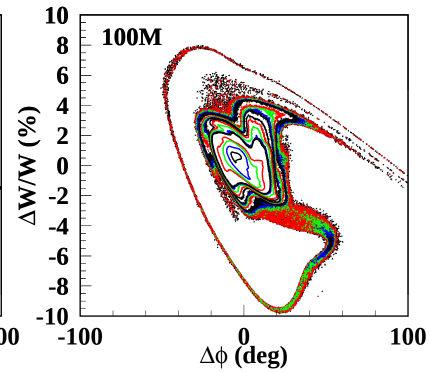
CPU	Time/cell (s)	Ideal Time (s)	Parallel Efficiency
512	384	384	100%
1024	225	192	85.3%
2048	107	96	89.7%
4096	63	48	76.1%

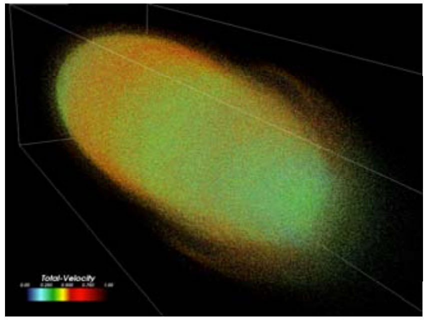
One to One RFQ Simulation: ~ 1 B particles

- Simulated the actual number of particles in 45 mA proton beam at 325 MHz accelerated in a RFQ from 50 keV to 2.5 MeV → 865 M particles on 32768 processors.
- Benefits of simulating a large number of particles: actual number if possible
  - Suppress noise from the PIC method: enough particles/cell
  - More detailed simulation: better characterization of the beam halo

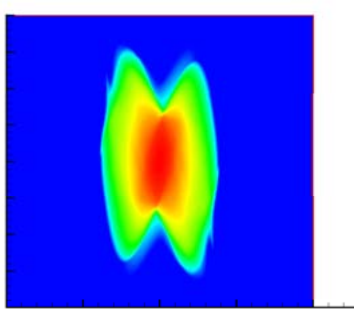




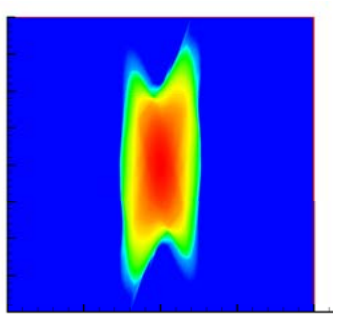




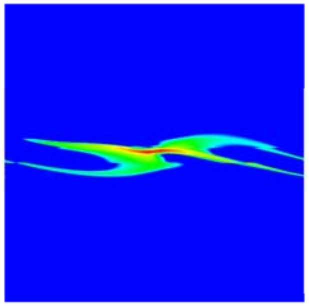
3D beam: 100M



(x, x')



(y, y')



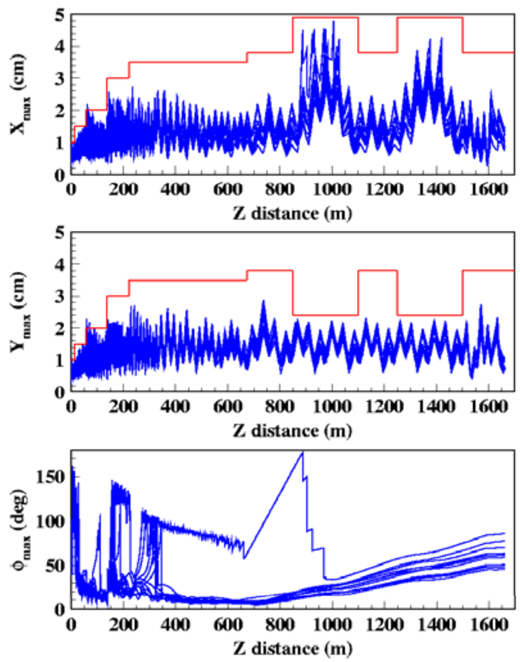
(Δφ, ΔW/W)

Phase space plots for 865 M protons after 30 cells in the RFQ.

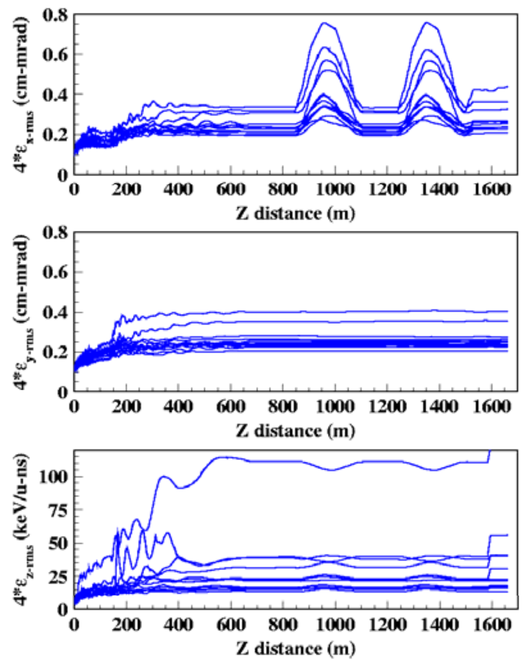
Large Scale Error Simulations: 10 M particles / seed

- Simulated machine errors with 10M particles per seed in the FNAL-PD linac:
  - ~ 2000 elements, 1.7 km long
  - misalignment errors and (1%, 1 deg) RF errors
  - includes H- stripping: Black body, residual gas and Lorentz stripping.
- Benefits of simulating a large number of particles/seed:
  - Study beam loss to the lowest possible level.

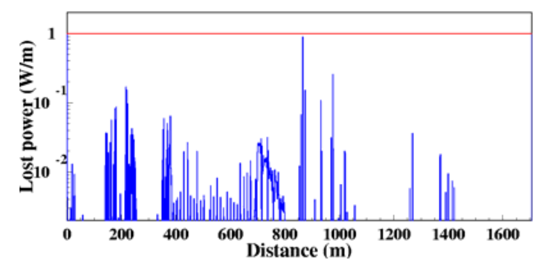
Envelopes



RMS emittances



Beam loss



Lost fraction: 9 E-4
Peak loss: 0.9 W/m

With H- stripping, the fraction lost increased by almost one order of magnitude → Linac & Transfer line should be cooled

Future Developments

- So far, the developed optimization tools were used only offline with the serial version of TRACK → Very time consuming.
- To be used online for real-time machine operations we should be able to perform large scale optimizations on large number of processors.
- The parallel version of TRACK is now ready, parallel optimizations are under development: New algorithms are being investigated.
- Develop more tools for the commissioning phase to tailor the computer model to the actual machine by fitting the measured data.
- Develop interfaces between the beam diagnostic devices and the beam dynamics code → Calibrate and analyze the data to input to the code.
- Numerical experiments may be used to test the tools before implementation into the real machine → Produce detector-like data from the code.
- Application to existing facilities …

Summary

- Developing a realistic computer model to support real-time accelerator operations should significantly improve its availability and reduce its operating cost.
- The realization of this concept of model driven accelerator requires a realistic 3D beam dynamics code with the appropriate set of optimization tools and large scale parallel computing capabilities.
- The beam dynamics code TRACK is being developed at Argonne to meet these requirements.
- Different optimization tools are needed for the different phases of an accelerator project, namely the design, commissioning and operations.
- For a new machine we should take advantage of the commissioning phase to bridge the gap between the original design and the actual machine by tailoring the computer model to the machine.
- More developments are needed to realize the model driven accelerator.

Suggestions to the Ion Linac Community

- Comparing data to simulations should be a routine → Push harder to understand the differences …
- Start thinking of developing realistic computer models for your high intensity linacs → Reduce beam loss and improve the machine availability
- Future projects:
  - Use more diagnostics or at least don't cut to fit the budget …
  - Try to avoid long structures where you can't insert diagnostic devices
  - Include a large scale computing facility to your project
- More diagnostic development is needed:
  - Transverse: Peak & Tail, 2D Profiles, Correlated 4D, …
  - Longitudinal: Better precision: Bunch length detectors, TOF systems…
  - …
  - May be invent a device that can do 6D at one shot ? Ha, Ha, Ha, …