TOWARDS A MODEL DRIVEN ACCELERATOR WITH PETASCALE COMPUTING*

B. Mustapha#, P.N. Ostroumov and J. Xu
Argonne National Laboratory, 9700 S. Cass Ave, IL 60439, U.S.A.

Abstract

Accelerator simulations still do not provide everything designers and operators need to deploy a new facility with confidence. This is mainly because of limitations preventing realistic end-to-end simulations of the beam from the source all the way through to a final interaction point and because of limitations in on-line monitoring that prevent a full characterization of the actual beam line. As a result, once a machine is built there can be a gap between the expected behavior of the machine and the actual behavior. This gap often corresponds to enormous work and significant delays in commissioning a new machine. To address the shortcomings of the existing beam dynamics simulation codes, and to fulfill the requirements of future hadron and heavy-ion machines, a starting point for a realistic simulation tool is being developed at ANL that will support detailed design evaluation and also fast turnaround simulations to support commissioning and operations. The proposed simulations will be performed on the fast growing computing facility at ANL with peta-scale capability.

MODEL DRIVEN ACCELERATOR: CONCEPT & MOTIVATIONS

Presently, no accelerator in the world could fully rely on a computer model for its operations. The main reason is a discontinuity between the design and operation phases. Many factors contribute to this discontinuity: 1-Simulations in the design phase assume almost perfect conditions and cannot reproduce the real machine, 2-Actual elements specification and performance are usually different from their original design and in most cases 3-Not enough diagnostic devices to characterize the machine. The lack of a realistic model to support the commissioning and operations results in significant delay in the deployment of a new machine and a lot of time spent on machine tuning during operations. This usually leads to low availability and high operating cost of the machine. For example, a complex project such as the proposed FRIB facility [1], where primary beams from proton to uranium up to 600 MeV/u are used to produce beams of rare isotopes all over the map, cannot afford not to have a computer model to support its operations.

We here propose to bridge the gap between the design and operation phases and develop a realistic model of the machine. Among the benefits of such a model is fast tuning for the desired beam conditions and fast retuning to restore the beam after a failure. This should significantly improve the availability of the machine and reduce its operating cost. The requirements for the development of such a model and the realization of the concept of the model driven accelerator are discussed in the next sections.

*This work was supported by the U.S. Department of Energy, Office of Nuclear Physics, under Contract No. DE-AC02-06CH11357.
mustapha@phy.anl.gov

REQUIREMENTS TO REALIZE THE MODEL DRIVEN ACCELERATOR

The main requirements for the realization of the model driven accelerator could be summarized in the development of a 3D beam dynamics code with the appropriate set of optimization tools and large scale computing capabilities. A multi-particle beam dynamics code is more realistic than matrix-based and single-particle codes because it supports 3D fields, includes fringe fields and appropriate space charge calculations. It also allows more detailed simulations necessary to study eventual beam loss and produce data similar to the measured data. Such a code should also include a large set of optimization tools. Optimization tools are needed not only for design optimization but also to tailor the computer model to the actual machine to be useful for real-time operations. Multi-particle optimizations usually involve tracking a large number of particles for large number of iterations which is very time consuming and requires large scale parallel computing. Therefore the beam dynamics code should have parallel computing capabilities.

The beam dynamics code TRACK [2] is being developed at Argonne to meet these requirements. TRACK and a selected set of applications will be presented in the next section.

A REALISTIC BEAM DYNAMICS CODE

The beam dynamics code TRACK is being developed over the last few years at the Physics Division of Argonne National Laboratory. Among the main features of TRACK are:

- A wide range of E-M elements with 3D fields
- End-to-end simulations from source to target
- Tracking multiple charge states heavy ion beams
- Interaction of heavy ion beams with strippers
- Automatic transverse and longitudinal beam tuning
- Error simulations: Static and dynamic errors
- Realistic transverse correction procedure
- Large number of particles for large number of seeds
- Beam loss analysis with exact location of the losses

And more recently:

- Possibility of fitting experimental data (profiles,…)
- H- Stripping: Black body, Residual gas and Lorentz

- The design and simulation of electron linacs
- Parallel version is fully developed with good scaling
- Simulating the actual number of particles in a bunch

A list of beam line elements supported by TRACK is given below:

- 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 or 3D fields)
- Dipoles with fringe fields (model or 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 extensively used in the design and simulations of the RIA/FRIB driver linac [3] and the FNAL-PD linac [4] and more recently in the end-to-end simulations of the SNS linac [5]. TRACK is now being used in the design and simulations of an electron linac for an X-FEL Oscillator [6].

Design and Simulations of the RIA/FRIB Linac

The physics design and the results of large scale beam dynamics simulations of the FRIB linac proposed by Argonne were presented and discussed in detail at a previous conference [3].

Design and Simulations of the FNAL-PD Linac

The physics design of the FNAL-PD linac was presented elsewhere [7]. Detailed beam dynamics simulations, including error and beam loss simulations for 100 seeds with million particles each, were presented at a previous conference [4]. The most recent results are presented in a separate paper at this conference [8].

End-to-end Simulation of the SNS Llinac

The results of the first end-to-end simulation of the SNS linac are presented in a separate paper at this conference [5].

Design and Simulations of an Electron Linac

Recently TRACK was used to design and simulate an electron linac for a future X-FEL Oscillator. This is discussed in more details in a separate paper at this conference [6].

VERSATILE OPTIMIZATION TOOLS

As discussed in the previous sections, the realistic beam dynamics code should also have the appropriate set of optimization tools to be used to support accelerator commissioning and operations. A set of optimization tools developed for TRACK are presented in this section. This tools could be easily adapted to other codes such as IMPACT [9].

Automatic Tuning Procedures

The automatic tuning procedures are developed to tune a given section of the linac to produce smooth beam dynamics by reducing the fluctuations in the rms beam size along a given linac section [10]. For the transverse tuning, the fit function is defined as:

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

where X^0_{rms} and Y^0_{rms} are the rms beam sizes at the entrance of the section, the sum index i runs over the focusing periods and ε_{Xrms} and ε_{Yrms} are the allowed errors on the rms beam sizes. The fit parameters are the field strengths in focusing elements. This method is general and should produce good results for periodic or non periodic accelerating structures. Applied for a two charge state uranium beam in the low-energy section of the RIA driver linac this method produced the results shown in Fig 1.

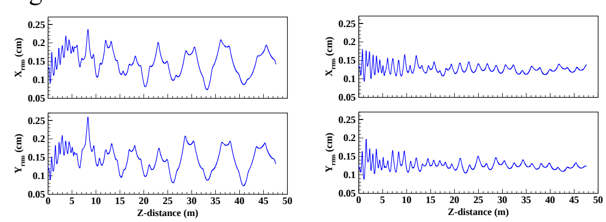

Figure 1: X and Y rms beam sizes before (left) and after (right) applying the automatic transverse tuning procedure. The beam is a two-charge state uranium beam in the low energy section of the RIA/FRIB driver linac.

Although developed for design optimization purpose this procedure could very well be applied to a real machine using beam profile measurements to reduce beam mismatch. A similar procedure was developed for the longitudinal rms envelopes.

Automatic Longitudinal FineTuning

A longitudinal fine-tuning procedure was developed specifically for a multiple charge state beam to minimize its longitudinal emittance right before a stripper [11]. The beam should reach the stripper in the form of an up-right ellipse in the (Δφ, ΔW) plane to minimize the emittance growth from the energy straggling effect in the stripper. This could be realized by matching the beam centroids and Twiss parameters of the different charge state beams. The fit function in this case is:

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

where W_0 is the desired beam energy and ε_W is the associated error. $\varepsilon_{\Delta W}$, $\varepsilon_{\Delta\varphi}$ and ε_α are the allowed errors on the relative energy, phase and α shifts of the individual charge state beams from the central beam. The fit parameters in this case are the RF cavities phases and amplitudes in the section up-stream of the stripper. Figure 2 shows the results of the fit for a five charge state uranium beam in the medium energy section of the RIA driver linac. This optimization reduced beam losses in the high-energy section of the linac by a significant factor.

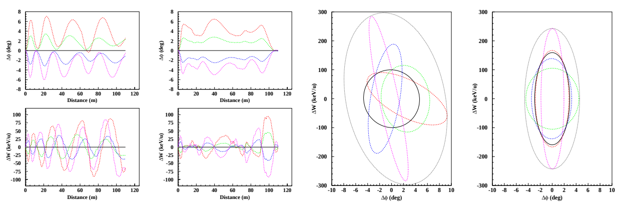

Figure 2: The left 4 plots show the phase and energy oscillations of the five charge states around the central charge state before and after applying the tuning procedure. The right 2 plots show the corresponding beam ellipses on the stripper before and after tuning.

This procedure could be used on a real machine but would require the measurements of energy and phase centers of individual charge state beams. More diagnostics development is needed to be able to measure and match the Twiss parameters.

Realistic Corrective Steering

A realistic corrective steering procedure was developed to correct for misalignment errors. The procedure uses virtual beam position monitors and correctors including measurement errors. It was applied for the front-end of the FNAL-PD linac to optimize the number and locations of monitors and correctors and to determine the required correctors field strengths and monitors precision. Figure 3 shows the appropriate set of monitors and correctors required in the front-end of the FNAL-PD linac. Figure 4 shows the results of the correction procedure along with the required corrector strengths.

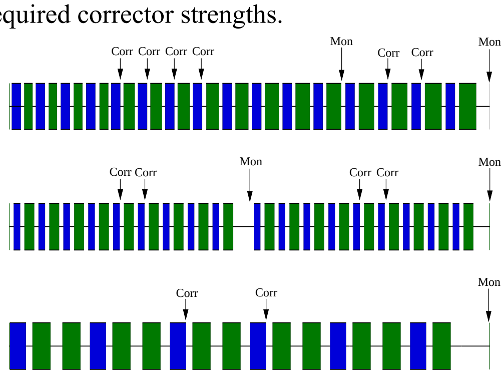

Figure 3: Monitors and correctors required for the front-end of the FNAL-PD linac.

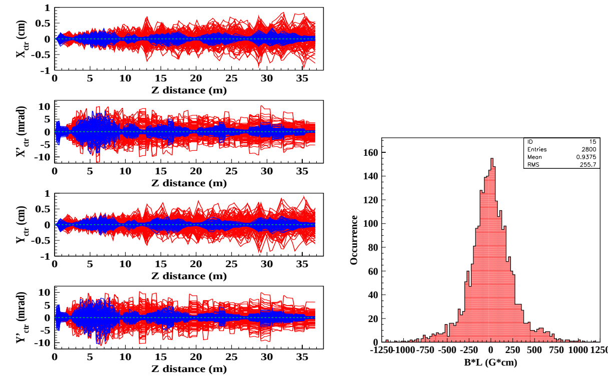

Figure 4: results of the correction procedure. On the right are beam centers in (x,x',y,y') before (red) and after (blue) correction. On the left is a distribution of required corrector strengths.

Figure 5 shows the effect of monitors precision on the correction procedure. The required precision should be 10-30 μ, much less than the misalignment error of 100 μ.

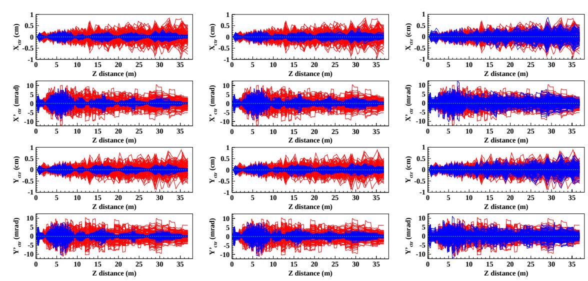

Figure 5: Effect of monitors precision on the correction: left: 10μ, middle: 30μ and right: 100μ.

This procedure could be easily implemented for a real machine using real beam position monitors and real beam steerers.

Operations of a Multi-Q Injector

New optimization tools have been developed to support the operations of the prototype multiple charge state LEBT at Argonne. By fitting the measured beam profiles we were able to determine the initial beam conditions at the source which were later used to find the appropriate quadrupole settings to recombine a two charge states 90 kV bismuth beam (20+, 21+) at the end of the LEBT. Figure 6 shows the result of the profile fit from which the beam emittance and Twiss parameters at the source are extracted. Figure 7 shows a TRACK fit to produce symmetric beam dynamics in the LEBT which is necessary to recombine the two charge state beams at the end of the LEBT. The quadrupole settings obtained from this fit was used on the actual beam line for an almost perfect recombination of the two beams. Figure 8 shows the measured profiles at the end of the LEBT for the individual and combined beams. Figure 9 shows a pepper-pot image of the combined beam and a superposition of individual charge state beam images.

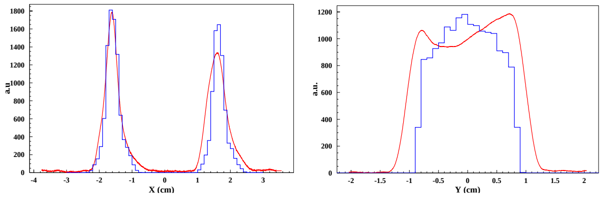

Figure 6: Horizontal (left) and vertical (right) beam profiles. The curves are the measured profiles and the histograms are the result of the TRACK fit.

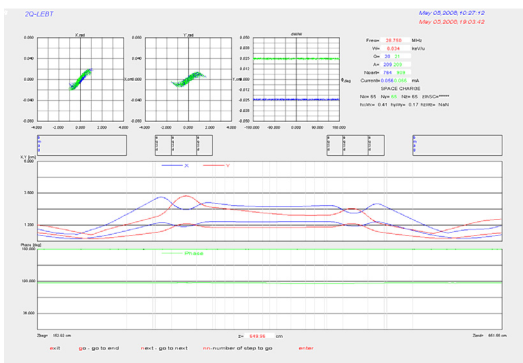

Figure 7: Result of a symmetric fit between the two LEBT magnets to recombine the two charge state Bi beams.

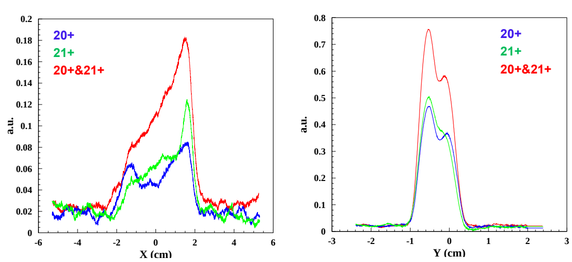

Figure 8: Measured beam profiles at the end of the LEBT for the individual Bi 20+ and 21+ beams and the combined beam.

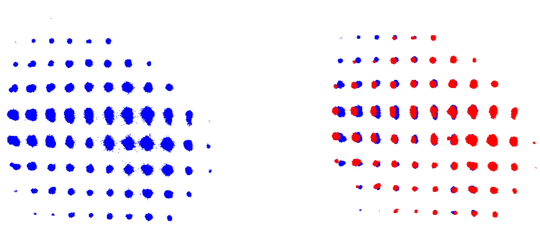

Figure 9: Pepper-Pot images of the combined beam (left) and the individual beams (right). Bi 20+ is in blue and 21+ is in red.

It is worth noting that without the support of the realistic TRACK simulations we would not be able to recombine the two charge state beams at the end of the LEBT.

LARGE SCALE PARALLEL COMPUTING

As mentioned above multi-particle optimizations require large scale parallel computing to be useful for real-time machine operations.

The beam dynamics code TRACK was recently parallelized and successfully used on world-class computing facilities. The parallelization method is described in more detail elsewhere [12]. More recently TRACK was used for the simulations of very large number of particles on up to 32768 processors with very good scaling [13].

One to One RFQ Simulations

We recently succeded to simulate the actual number of particles in a 45 mA proton beam bunch at 325 MHz accelerated in a RFQ from 50 keV to 2.5 MeV. That is 865 million particles simulated on 32768 processors in 6 hours on the Blue-Gene machine at Argonne. The benefits of simulating a large number of particles is first to suppress the noise from the PIC method with enough particles per cell and second to better characterize the beam especially halo formation. Figure 10 shows phase space plots in the RFQ for 865 M particles.

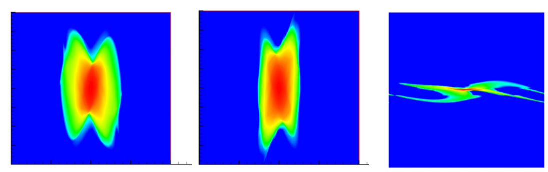

Figure 10: Phase space plots after 30 cells in the FNAL-PD RFQ. Left (x,x’), middle (y,y’) and right (Δφ,ΔW/W).

Error Simulations With Large Number of Particles

We simulated machine errors with 10M particles per seed in the FNAL-PD linac and transfer line with ~ 2000 elements and 1.7 km long. Included are misalignment errors and RF errors of (1%,1 deg) as well as H- stripping by three different processes, namely, black body radiation, residual gas interaction and Lorentz stripping. The benefit of simulating a very large number of particles is to study beam loss to the lowest possible level. Figure 11 shows beam envelopes and emittance for multiple seeds and Fig. 12 shows the beam loss in Watts/m along the linac.

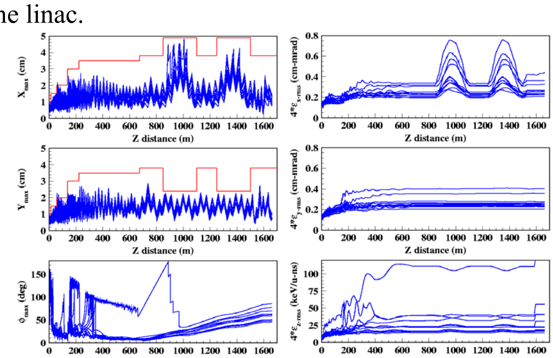

Figure 11: Beam envelopes (left) and emittances (right) along the FNAL-PD linac and transfer line for multiple seeds.

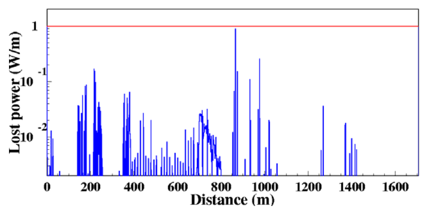

Figure 12: Beam loss in Watts/m in the FNAL-PD linac and transfer line. In red is the conventional 1 W/m limit.

We notice that by adding the H- stripping, the losses increased by an order of magnitude which suggest that the transfer line should be cooled to reduce the stripping by black body radiation.

FUTURE DEVELOPMENTS

The tools developed so far were used only offline with the serial version of TRACK which is 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 (32768 processors or more). The parallel version of TRACK is now fully developed and scales reasonably well on very large number of processors. Parallel optimizations are now under development. We are investigating new parallel optimization algorithms such as the Toolkit for Advanced Optimization (TAO) developed at the Mathematics and Computer Science Division at Argonne [14].

More optimization tools need to be developed for the commissioning phase to tailor the computer model to the actual machine by fitting the measured data. For this purpose, interfaces between the beam diagnostic devices and the computer model are needed to calibrate and analyze the data to input to the code. Numerical experiments could be used to test and fine tune the tools before implementation to the real machine by producing detector-like data. Only after all these developments we can actually realize the model driven accelerator. As a full scale application, we are proposing to apply this concept to the superconducting linac ATLAS at Argonne and to other existing machines as a preparation exercise for the future FRIB facility.

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 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 to the machine. More developments are needed to realize the concept of the model driven accelerator.

REFERENCES

[1] N. Ostroumov et al, Proceedings of PAC-07 Conference, Albuquerque, New Mexico, June 25-29, 2007.
[2] V.N. Aseev et al, Proceedings of PAC-05 Conference, Knoxville, Tennessee, May 16-20, 2005.
[3] B. Mustapha, P.N. Ostroumov and J.A. Nolen, Proceedings of PAC-07 Conference, Albuquerque, New Mexico, June 25-29, 2007.
[4] P.N. Ostroumov, B. Mustapha and V.N. Assev, Proceedings of LINAC-06 Conference, Knoxville, Tennessee, August 21-25, 2006.
[5] B. Mustapha et al, this conference
[6] P.N. Ostroumov et al, this conference
[7] P.N. Ostroumov, V. N. Aseev, and A.A. Kolomiets, J. of Instr., JINST 1, P04002, 2006
[8] P.N. Ostroumov et al, this conference
[9] J. Qiang, R. D. Ryne, S. Habib, and V. Decyk, J. Comput. Phys. 163 (2000) 434.
[10] B. Mustapha and P.N. Ostroumov, Proceedings of LINAC-06 Conference, Knoxville, Tennessee, August 21-25, 2006.
[11] B. Mustapha and P.N. Ostroumov, Phys. Rev. ST. Accel. Beams 8, 090101 (2005).
[12] J. Xu, B. Mustapha, V.N. Aseev and P.N. Ostroumov, Phys. Rev. ST. Accel. Beams 10, 014201 (2007).
[13] J. Xu, B. Mustapha, V.N. Aseev and P.N. Ostroumov, Proceedings of the HB-2008 Workshop, Nashville, Tennessee, August 25-29, 2008.
[14] S. Benson, L. McInness, J. More, T. Munson and J. Sarich, "TAO User Manual (Revision 1.9)", Mathematics and Computer Science Division, Argonne National Laboratory, ANL/MCS-TM-242, and at http://www.mcs.anl.gov/tao.