CHALLENGES OF RECONCILING THEORETICAL AND MEASURED BEAM PARAMETERS AT THE SNS ACCELERATOR FACILITY
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Abstract
The Spallation Neutron Source (SNS) is steadily approaching its design beam power of 1.4 MW without encountering major of the models used for the accelerator design and tuning. Nevertheless, it is surprisingly difficult to reconcile many of the measured beam parameters with the model prediction. In this paper we discuss several examples of such discrepancies, ranging from a simple single particle tracking to beam emittance measurements. We also present our approach to resolving some of the issues from a diagnostics standpoint.

INTRODUCTION
The intention of this talk was to initiate a discussion during a joint session of the Computational Challenges and the Beam Diagnostics and Instrumentation working groups on the issues of reconciling measured beam parameters with computer simulations. This topic is not new and has been a subject of intense discussion during every HB workshop.

The SNS accelerator, recently commissioned, is one of the newest and highest intensity proton machines in existence. Advanced computer simulation tools were used during its design, and it is equipped with a comprehensive set of beam diagnostics. This makes the SNS accelerator a practical, state-of-the-art example for reconciliation of high intensity beam simulation with measurements. Due to length limitations we will only discuss problems related to the SNS linac in this document.

The SNS is running at 1 MW and no problems are expected up to the design beam power of 1.4 MW. This success is a confirmation of the general validity of the models used for the accelerator design and tuning. At the same time, our commissioning and initial operation experience shows that it is surprisingly difficult to reconcile many of the measured beam parameters with the model predictions. The important questions to ask are: Are the models we used as design tools capable of predicting major beam parameters in the operational accelerator? If yes, are they accurate and powerful enough to predict beam loss? Do we need to have such accurate models? If yes, do we believe it is realistic to obtain such a high level of accuracy, should we even try? We can not give answers to these questions in this document but will provide some practical examples to illuminate several aspects of the problem: The accuracy of the models, the reliability of the measured data, the uncertainty in the knowledge of the machine state and the initial distribution.

BEAM DYNAMICS SIMULATION
There are many computer codes available these days powerful code PARMILA was the main simulation tool for the SNS linac design. Some other codes were used for simulation of beam dynamics in linear and circular accelerators. Some of them can run on parallel computers and track tens of millions of particles with 3D space charge calculations. An older and less for verification of the design stability and for error tolerance studies, such as IMPACT, LINAC and TRACE-3D. End-to-end simulations with different initial distributions demonstrated good agreement between the codes. Expectations have been high, based on quick and successful commissioning of the linac, that the same models can accurately predict the beam parameters in the real accelerator, maybe even beam halo and losses. These expectations have not materialized so far, and there is a growing understanding that a different kind of computer model is required for predicting behavior of real beams in real accelerators.

A real machine is characterized by a very large number of parameters, the precise values of which are not known. A few examples are RF phases and amplitudes, magnet strengths and offsets, etc. A common practical way to determine these values is to fit the model to the available experimental data by varying the parameters of interest in the model. To solve this optimization problem a large number of runs are required, preferably in real time with live data in the control room. This is unrealistic for end-to-end simulations with large numbers of particles and 3D fields, even with modern computing capabilities. But this is exactly the modern trend in simulation code development: End-to-end simulations with huge numbers of particles and 3D-field calculations. The motivation for increasing the number of simulated particles and mesh density is to increase the accuracy of electro-magnetic field calculations, which defines the final accuracy of particle motion in the model. This is the correct approach for modeling an ideal accelerator. But in a real machine, very often the model accuracy is defined by knowledge of the actual hardware parameters, and therefore increasing the number of simulated particles and the mesh density does not improve the accuracy of the model predictions. As a result of growing computer power requirements for modern accelerator design codes, it becomes impractical to use them for real machine simulation. In practice we have to use a combination of codes or pieces of codes for modeling different aspects of beam dynamics in different portions of the SNS linac. At present, these pieces are not connected and there is no convenient framework for the data analysis with good optimization capabilities.
Table 1 illustrates the current state of agreement between beam dynamics simulations and measurements for the SNS linac. The rows of the table correspond to the different sections of the linac, and the columns correspond to different aspects of the beam dynamic. In principle, every cell in the table can represent a separate code. The terms: “bad”, “good”, and “very good”, qualifying accuracy of the models in the table, are informal and not well defined. We will give examples of their meaning in the next sections. It should be noted that this table mainly reflects the author’s personal opinions, and changes continuously as models evolve. As one can see from the table, we cannot reliably simulate even the motion of the beam center of gravity in some segments of the linac. Is it realistic, then, to expect a reliable simulation of the beam envelope, not to mention the halo?

Table 1 Beam Modeling Accuracy in the SNS Linac

<table>
<thead>
<tr>
<th></th>
<th>Transv. centroid</th>
<th>Transv. RMS</th>
<th>Long. centroid</th>
<th>Long. RMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>RFQ</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>MEBT</td>
<td>good</td>
<td>good</td>
<td>not so good</td>
<td>good</td>
</tr>
<tr>
<td>DTL</td>
<td>good</td>
<td>not so good</td>
<td>very good</td>
<td>NA</td>
</tr>
<tr>
<td>CCL</td>
<td>very good</td>
<td>not so good</td>
<td>very good</td>
<td>not so good</td>
</tr>
<tr>
<td>SCL</td>
<td>not so good</td>
<td>not so good</td>
<td>very good</td>
<td>NA</td>
</tr>
</tbody>
</table>

**BEAM DIAGNOSTICS**

Beam measurements play a very important role in creating a realistic beam model. As we discussed in the previous section, they are used not only to validate the model but to find the essential model parameters. Therefore the achievable model quality depends strongly on the quality, specifically the accuracy and resolution, of the beam instrumentation.

The number of measurement stations and the speed of taking data are also important, because in practice a large number of measurements are required to constrain the fitted parameters with a good accuracy, especially if the diagnostics are scarcely distributed.

A good simulation framework should have a capability for efficient manipulation and analysis of large volumes of beam diagnostics data.

The beam instrumentation must have reliable verification tools as well. As we will show in the examples below, a trustworthy model can reveal systematic errors in the measured data.

**SNS LINAC EXPERIENCE**

In this section we will show, using examples from the SNS linac commissioning experience, how computer simulations of various aspects of the beam dynamics compare with the measurements.

**Longitudinal Motion of Beam Center of Gravity**

A comparison between the calculated and the measured beam phase deviation from the reference phase along the SNS CCL is shown in Fig. 1. This level of agreement is called “very good” in the Table 1, and is achieved by using an iterative procedure of tuning the CCL RF amplitude and adjusting the model parameters. The same model does not always work well in other segments of the linac, as illustrated by Fig. 2, where a typical MEBT re-buncher phase scan plot is shown. According to the “single particle” model, the intersection points of the lines on the graph should be at the same phase for all BPMs. The measurements give a phase difference of several degrees between the two BPMs (this is an example of a “not so good” agreement in the Table 1). This discrepancy cannot be explained within the framework of “single particle” dynamics. Asymmetry of the beam distribution function is a plausible explanation, but it has not yet been confirmed by PIC code simulations.

Figure 1: Phase oscillations in the SNS warm linac (solid line – model; blue points - experiment).

Figure 2: Phase scan of the SNS MEBT re-buncher cavity.

The first example demonstrates that even a very simple model can describe some important aspects of the beam dynamics with high accuracy. Such models are very efficient; they can and should be used for machine tuning and for finding the important model parameters. The second example demonstrates that there are limits of validity, beyond which more complicated models have to be used. A beam measurement is a good tool for finding these limits.
Transverse Motion of Beam Center of Gravity

The vertical beam trajectory in the SNS CCL, after correcting it using the two different models, is shown in Fig. 3. This is another example of “very good” agreement in Table 1. The original model (labeled “old model” in the picture) did not describe the beam center of motion very well. The discrepancy between the model, which predicts exactly zero displacement everywhere, and the measurements, shown by the red dots on the graph, can reach up to ±6mm. In order to improve the model we introduced transverse offsets in the quadrupole magnets, which are optimized to achieve the best agreement with the multiple sets of measurements. The discrepancy was reduced by a factor of three and is comparable with the accuracy of the measurements. Unfortunately, the offsets we had to include in the model do not agree with the magnet position measurements and, generally, are too large to be real. This is an example of a not entirely correct model providing high accuracy. There is something in the real machine we do not understand, but we can mimic overall effect of that “something” using the artificial quad offsets. This approach is effective for modeling the transverse motion of the beam center. It remains to be proven by more measurements if it will work for other beam parameters, such as the rms beam size.

Figure 3: Corrected vertical beam trajectories in the SNS CCL, after correction using the two different models.

Transverse rms Beam Size

We can reproduce the transverse rms beam size in some segments of the linac reasonably well, as illustrated by the plot on the left side in Fig. 4. The input Twiss parameters in this case are found by searching for the values which minimize the difference between model and measurement. If the parameters of the focusing elements in the beam line are changed then the beam envelope changes, but the input Twiss parameters should stay the same. The results of such an experiment are shown on the right side of Fig. 4. The set of the squares on the plot represent input Twiss $\alpha$ and $\beta$ optimized for different sets MEBT focusing configurations. There is some spread of the Twiss parameters due to inaccuracy of the measurements and/or of the model. There is, also, a significant difference with the expected values for the vertical parameters, predicted by the model of the upstream RFQ (shown by large circles). This is a good example of the old problem of defining the initial input parameters for simulation. It also illustrates the weakness of the usual approach in end-to-end simulations, when measured parameters at the source are propagated down the machine. If there is a inaccurate model anywhere in the chain (the RFQ model in our example), then all downstream results become inaccurate.

Figure 4: Transverse rms beam size in the SNS MEBT.

Figure 5a: Measured transverse emittance in the MEBT.

Figure 5b: Simulated transverse emittance in the MEBT.

Figure 6: Measured dependence of the rms emittance vs. the re-buncher RF phase.
Longitudinal rms Beam Size.

The longitudinal bunch size has a significant effect on the beam dynamics in a linac due to the RF field dependence on the RF phase and the space charge force dependence on the charge density. Longitudinal diagnostics are usually scarce, and therefore the longitudinal beam parameters often have to be assumed. It makes the available longitudinal measurements very important for validating the initial beam distribution assumptions and the model accuracy. A comparison between the measured and the simulated bunch length in the SNS CCL is shown in Fig. 7. The initial Twiss parameters in the model are optimized for the best agreement with the measured data, separately for each location of the longitudinal profile monitor. This example shows that a very good agreement can be achieved with properly selected initial parameters. An attempt to fit the model to the measurements at four points simultaneously is less successful, as shown in Fig 8. The three measured points are reproduced well by the model, but the fourth point is off. The beam size oscillations, visible on the plot, suggest that there is significant mismatch at the CCL entrance, if true. But these measurements are made at the limit of the available diagnostics resolution and there is no confidence in their accuracy. There is no confidence in the model accuracy either, because the only way to validate the model is to compare it with reliable measurements. The most straightforward way to resolve this uncertainty is to increase the diagnostics resolution and accuracy.

SUMMARY

We have demonstrated using examples from the SNS linac commissioning experience, that problem of reconciliation between simulations and measurements extends beyond a correct representation of the electromagnetic fields and an accurate tracking. The actual parameters of the real machine have a significant degree of uncertainty. One possible way to find these parameters is to minimize the difference between the model and the beam measurements by varying the parameters. In other words, the model is adjusted to fit the measured data. An optimization problem with many variables requires many constraints to converge reliably. This entails measurements of multiple beam properties: transverse, longitudinal, center of mass, rms size, profiles, phase advance, etc. New computer codes, different from the codes used for the accelerator design, are required for efficient use of these data. They must be flexible and have efficient optimization tools. The diagnostics need to be numerous, accurate and fast. These requirements are challenging but not impossible, considering the enormous progress in computer science and digital electronics in recent years.

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