The impact of phase space correlations on the beam dynamics in a linear accelerator

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2024-10-13

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Almost one year ago, CERN hosted the "68th ICFA Advanced Beam Dynamics Workshop on High-Intensity and High-Brightness Hadron Beams", also known as "HB". I gave a talk on our work at the SNS Beam Test Facility (BTF). I intended to share that work on this blog, but never got around to it. Better late than never:

The initial beam

I usually start these talks by reviewing the LEDA (Low Energy Test Accelerator) experiment at Los Alamos National Laboratory Allen et al. (2002). LEDA was a proton source followed by 50 quadrupole magnets arranged in an alternating focus-defocus pattern (FODO). A series of experiments recorded the one-dimensional particle distribution different sets of quadrupole strengths. In some cases, simulations reproduced the measurements in regions of high particle density, i.e., the beam core. But no simulation reproduced the low-density "tails" or "halo".

Halo formation is driven by space charge (electric forces between particles). Thus, the discrepancies might have been due to an inaccurate initial distribution in 6D phase space. (They only estimated second-order moments.) On the other hand, errors in the accelerator model might have been to blame. Reproducing halo-level features requires modeling a delicate interplay between applied and self-generated fields.

At the BTF, we're trying to improve on LEDA's results. Our primary advantage is a suite of novel phase space diagnostics. One of these diagnostics images the 6D phase space distribution

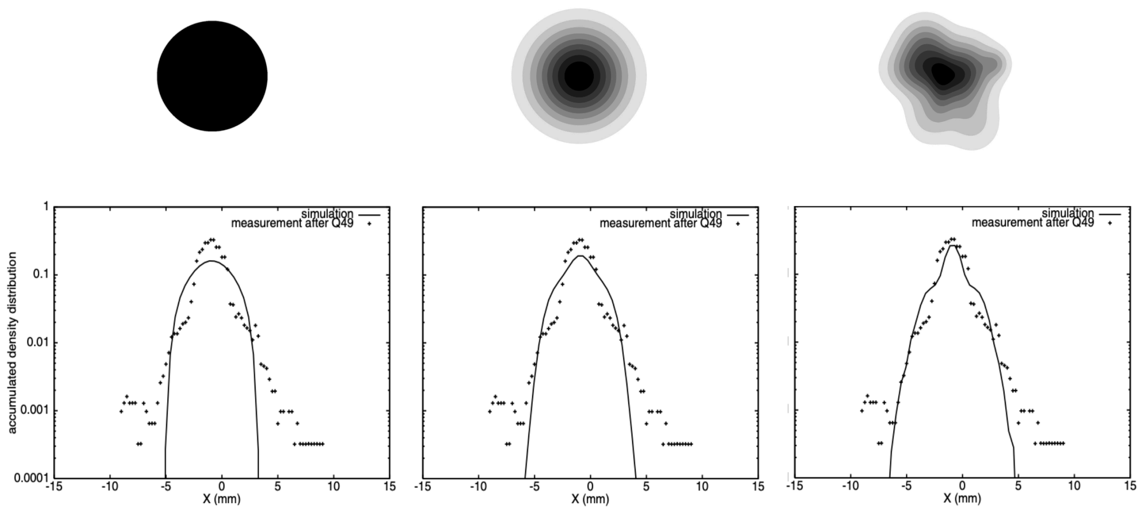

Figure 1: Measured and simulated beam profiles in the LEDA experiment Qiang et al. (2002).

at the beginning of the lattice Cathey et al. (2018). Another diagnostic measures the beam halo in 2D phase space at the end of the lattice Aleksandrov et al. (2021). In the first half of my postdoc, I focused on measurements of the initial distribution: see conference reports here and here. We observed major differences between our predictions at the end of the beamline and our predictions at the start of the beamline. One culprit could have been the paperclip layout of the BTF. Bending 180 degrees generated dispersion in the beamline, and we were unsure if we were modeling the dipole magnets correctly. In any case, linacs are typically straight lines, so we upgraded the BTF to a new straight layout. This took several months.

In the meantime, I examined a question that could be partially answered by computer simulations: How important is the initial 6D phase space structure? What if we ignore correlations between certain dimensions? An easy way to answer this question is to use the measured 6D distribution. However, 6D measurements currently have low resolution ($\approx 10^6$ points), and low dynamic range ($\approx 10^1$), and it's unclear if this is sufficient to predict anything about the halo at the end of the beamline.

There's another way to generate the initial beam which avoids direct 6D measurements. The initial beam is not really the initial beam; it's the beam at the location labeled "First Emittance Station" in Figure 2.

The beam emerges from the ion source as a continuous stream of ions. The RFQ (Radio Frequency Quadrupole) accelerates the beam to 2.5 MeV and converts the continuous stream to a train of short *bunches*. Before the RFQ, the longitudinal distribution is spatially uniform with a tiny energy spread; thus, defining the initial beam would only require a 4D (transverse) phase space measurement. However, we would then need to simulate the journey through the RFQ, which involves complex dynamics over hundreds of focusing periods with strong space

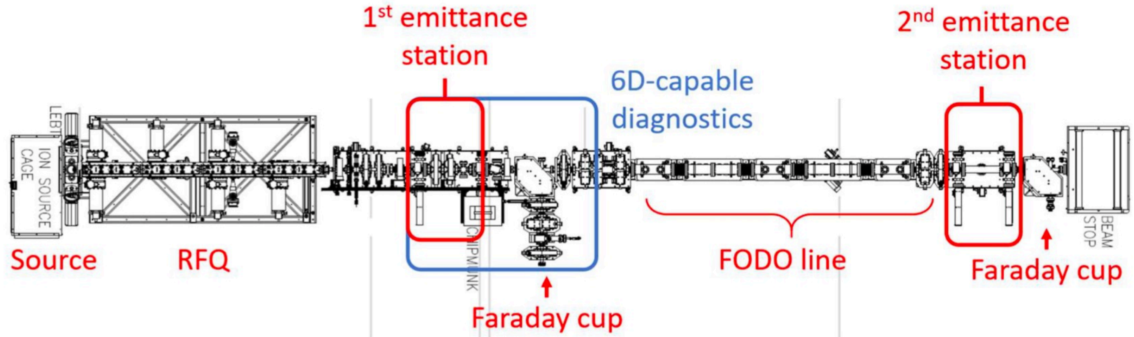

Figure 2: The SNS Beam Test Facility (BTF).

charge. So, we opted for a more difficult measurement after the RFQ.

Still, we could try this approach. We don't have any diagnostics before the RFQ (there's no room), but we do have 2D diagnostics at a dedicated Ion Source Test Stand. The ion source is different from the one in BTF, but it should produce a similar distribution. We took some old measurement data of a 50 mA beam in the Ion Source Test Stand and tracked it through the RFQ. The RFQ code (PARMTEQ) predicted 42 mA beam current, but the real RFQ generated around 26 mA. That's a huge unexplained discrepancy! We're still unsure what caused this because we can't peer inside the RFQ. Unphased, we artificially changed the bunch current to 26 mA in the simulation and tracked it to the first measurement station in the BTF.

PARMTEQ vs. reality

The PARMTEQ simulations generate a fully correlated 6D bunch without a direct measurement. The tradeoff is that we're unsure how realistic this distribution is. We know PARMTEQ gets the basic physics correct, but the model contains various approximations, such as an assumed cylindrical symmetry when solving the Possion equation. The only way to know is to compare it to direct measurements.

A previous paper found reasonable agreement in high-dimensional slices Ruisard et al. (2020), and I set out to perform a more comprehensive comparison. We have already performed 5D measurements of the initial beam, mapping the density as a function of x, p_x, y, p_y, and p_z Hoover et al. (2023). The missing dimension, z, is strongly correlated with p_z, so most features are visible from the five measured variables. 5D measurements are much faster than 6D measurements because we can image two dimensions at once on a screen (and because there is one less dimension to measure). Because of the boosted resolution and dynamic range, we can visualize sharper features in low-density regions of phase space.

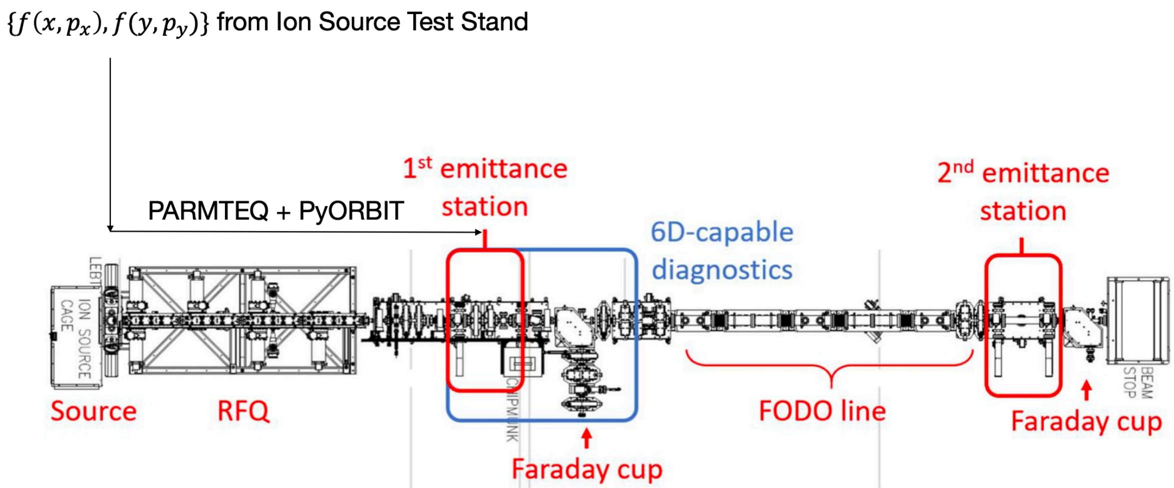

Figure 3: PARMTEQ model bunch generation. An initial 2D measurement is transported through the RFQ using PARMTEQ and through the first section of the BTF using PyORBIT.

Here are the 1D and 2D projections of the measured and predicted (PARMTEQ) distributions. Note that I use $x' = p_x / p_z$ and $y' = p_y / p_z$ for the transverse momentum. I also use w instead of p_z, where $w = E - E_0$ is the deviation from the design energy.

These contours are on a logarithmic scale, showing three orders of magnitude in density. It's is not a total disaster, but it's kinda bad. Particularly troublesome is the x-p_x distribution, which is much wider than measured. However, look what happens after a linear transformation:

Much better! All I did was normalize both distributions to identity covariance so that

$$\Sigma = \begin{bmatrix} \langle xx \rangle & \langle xp_x \rangle & \langle xy \rangle & \langle xp_y \rangle & \langle xp_z \rangle \\ \langle xp_x \rangle & \langle p_x p_x \rangle & \langle yp_x \rangle & \langle p_x p_y \rangle & \langle p_x p_z \rangle \\ \langle xy \rangle & \langle yp_x \rangle & \langle yy \rangle & \langle yp_y \rangle & \langle yp_z \rangle \\ \langle xp_y \rangle & \langle p_x p_y \rangle & \langle yp_y \rangle & \langle p_y p_y \rangle & \langle p_y p_z \rangle \\ \langle xp_z \rangle & \langle p_x p_z \rangle & \langle yp_z \rangle & \langle p_y p_z \rangle & \langle p_z p_z \rangle \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{1}$$

From now on, I'll let x, p_x, y, p_y, and p_z refer to these "normalized" coordinates. Figure 5 shows that the distributions are similar, up to a linear transformation. PARMTEQ has gotten the nonlinear stuff right, even though it predicts a much larger transmission than measured in the real RFQ. This suggests that losses occur very early in the bunch formation process and have little impact on the higher-order distribution moments.

Figure 5 does *not* prove that the distributions are identical in the full five-dimensional space. There are two higher-dimensional correlations we've identified in our 5D measurement. First,

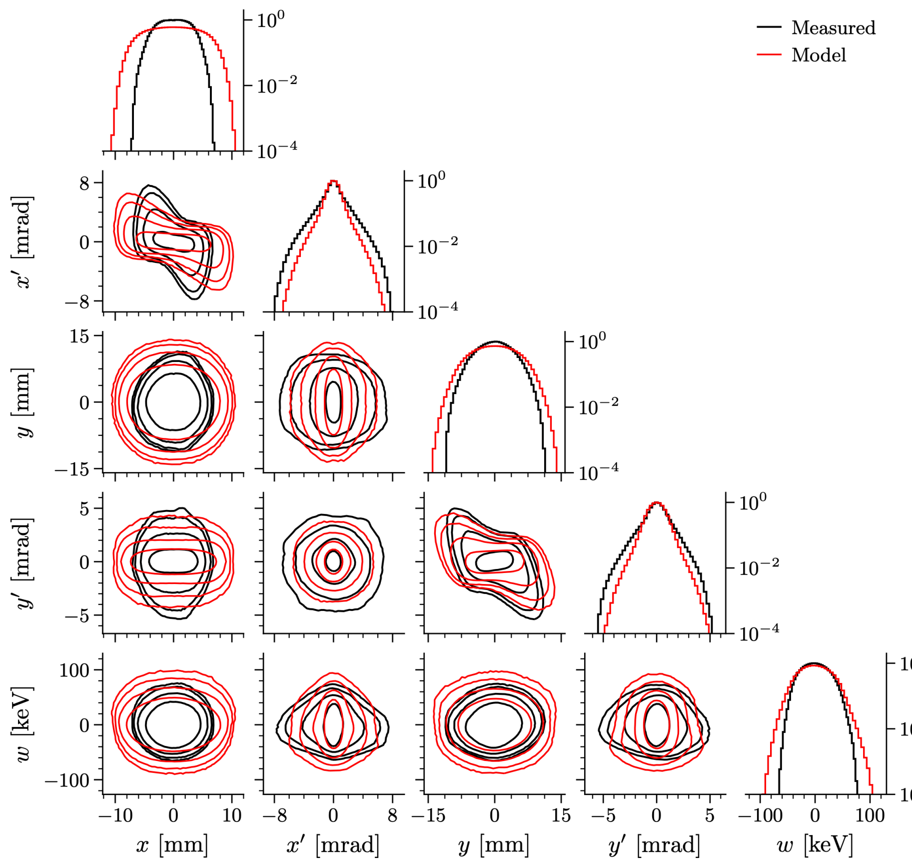

Figure 4: Measured (black) and predicted (red) phase space distributions in the BTF.

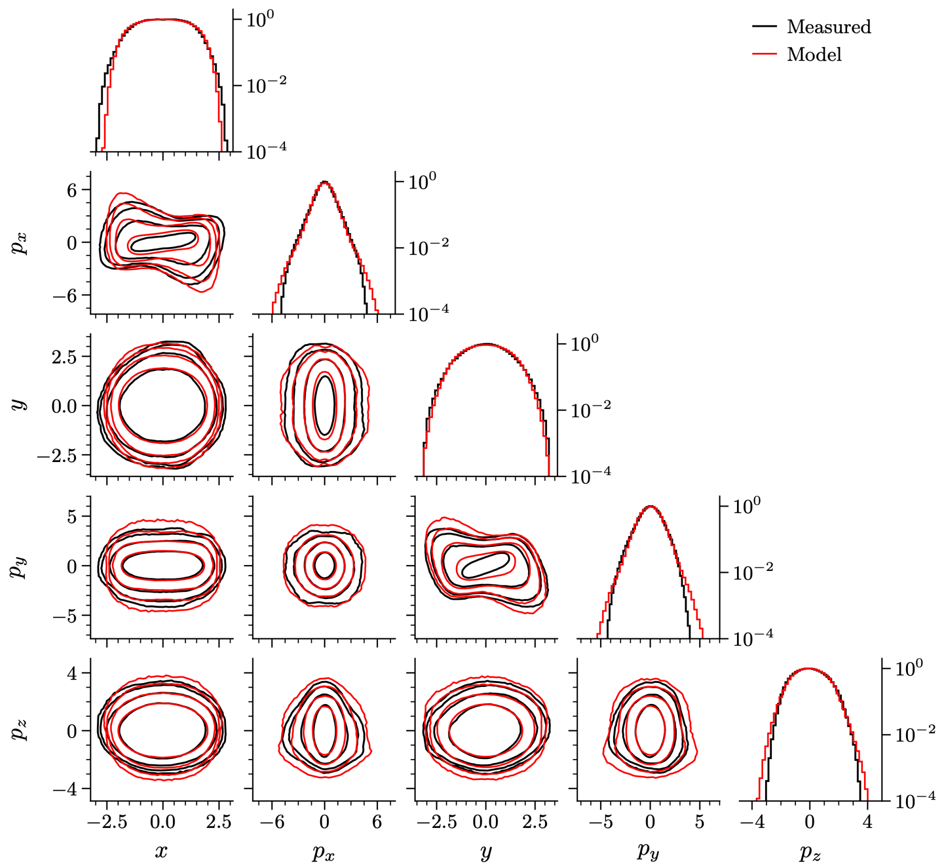

Figure 5: Normalized phase space distribution.

we know the energy distribution (p_z) depends on the transverse coordinates. The energy distribution is bimodal near the transverse core but unimodal outside the core. You can't see this in the 1D and 2D projections. One way to visualize the relationship is to use "elliptical slices". Figure 6 shows the $p-z$ distribution of particles within a radial band in x-p_x-y-p_y space. The model bunch has the correct relationship between energy and transverse radius.

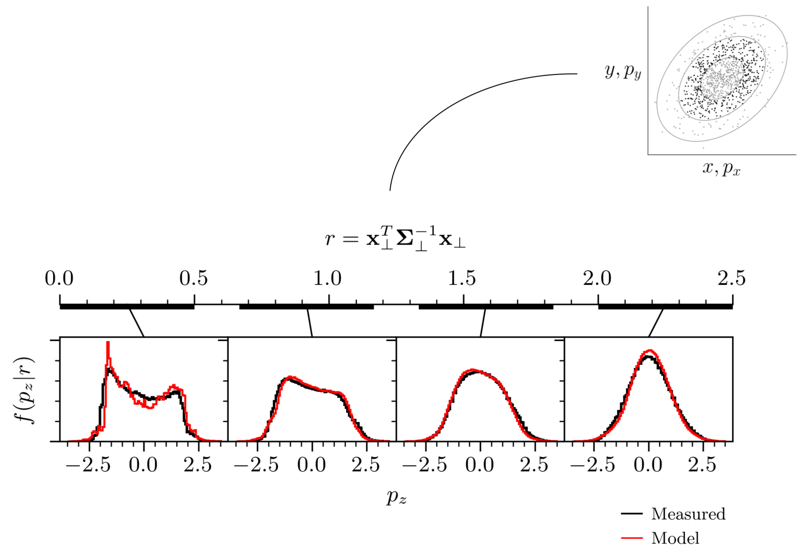

Figure 6: Energy distribution within ellipsoidal shells in the transverse plane.

The above feature develops somewhere in the RFQ. We've also measured hollowing in the 3D space x-y-z. This feature develops after the RFQ. As the beam transitions from strong to weak focusing at the RFQ exit, space charge launches a density wave that flattens the initially peaked distribution to a more uniform and, eventually, hollow distribution. The beam freely expands in the longitudinal plane, creating a strong linear correlation such that ($z \approx p_z$). Again, we see similar features in the model bunch. We conclude that the RFQ simulation reproduces nearly all measured features in both low-dimensional and high-dimensional phase space, up to a linear transformation.

Is 6D structure important in the SNS linac?

The above result is interesting and not too obvious; I'd like to include it in a future publication alongside a more detailed study of the beam dynamics in the RFQ. The result is also useful because linear correlations are easy to measure. We can just map the PARMTEQ bunch to the measured linear correlations, and, *voila*, we have a fully correlated 6D bunch that should be very similar to the real bunch.

We can also use this model bunch to examine what could happen in the SNS linac. Predicting beam loss in the SNS is our ultimate goal. This is way harder than our task in the BTF: the

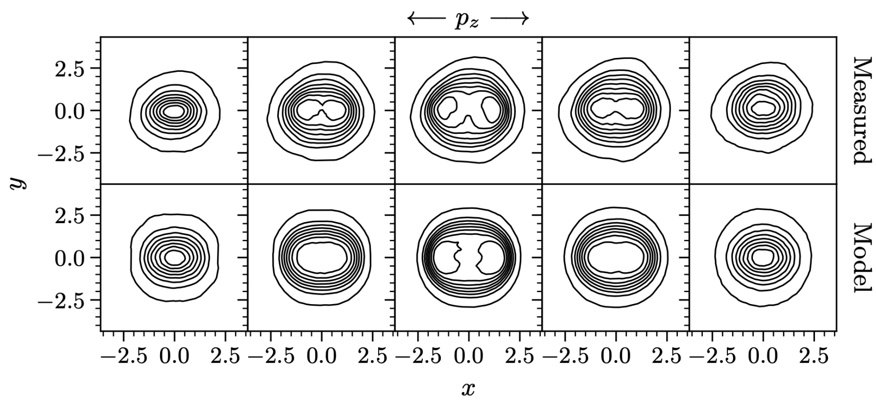

Figure 7: Transverse charge distribution (x-y) as a function of energy (p_z).

SNS is around 500 meters long compared to 10 meters in the BTF; the SNS accelerates the beam using hundreds of RF cavities, while the BTF has no acceleration; we are much less certain about the accelerator parameters; etc. Figure 8 gives a sense of scale. Still, we can assume our linac model is correct and see how different initial beams behave. This must tell us *something*.

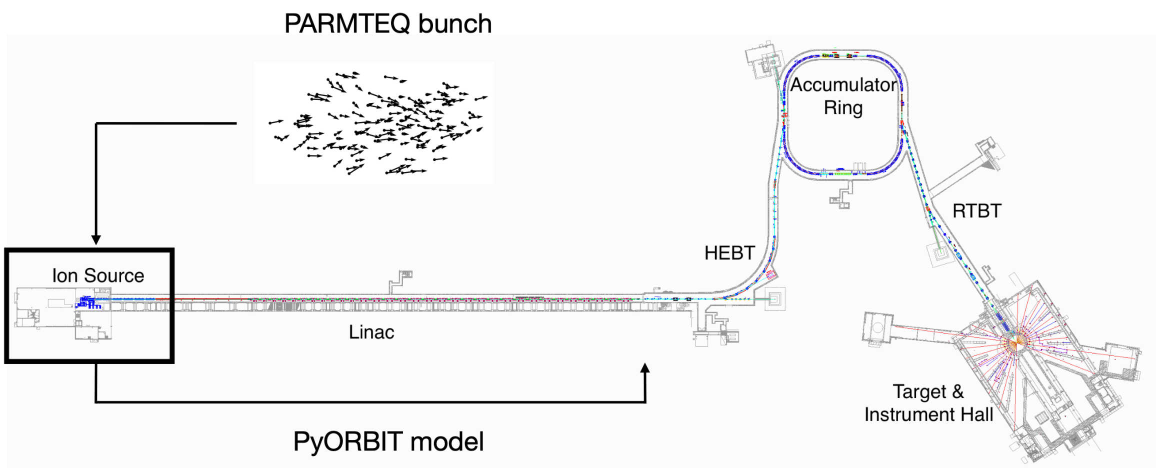

Figure 8: Diagram of the SNS accelerator. The linac is around 400 meters long.

We treated our PARTMEQ bunch as the ground truth. We then *decorrelated* the three planes:

$$
\begin{aligned}
\{x_i, p_{x_i}\} &\rightarrow \{x_i, p_{x_i}\}, \\
\{y_i, p_{y_i}\} &\rightarrow \{y_j, p_{y_j}\}, \\
\{z_i, p_{z_i}\} &\rightarrow \{z_k, p_{z_k}\},
\end{aligned} \tag{2}
$$

where i, j, and k are random permutations of the particle indices. The resulting distribution is a product of the 2D distributions:

$$
f(x, p_x, y, p_y, z, p_z) = f(x, p_x) f(y, p_y) f(z, p_z). \tag{3}
$$

All cross-plane correlations, including higher-order correlations, vanish in the decorrelated bunch. Then we tracked these two bunches (correlated and decorrelated) through the linac in our PyORBIT model and compared the trajectories.

This isn't new. My colleague did this in 2021, finding that the two beams diverged in their rms sizes (Figure 9).

12th Int. Particle Acc. Conf. IPAC2021, Campinas, SP, Brazil JACoW Publishing
ISBN: 978-3-95450-214-1 ISSN: 2673-5490 doi:10.18429/JACoW-IPAC2021-THXA01

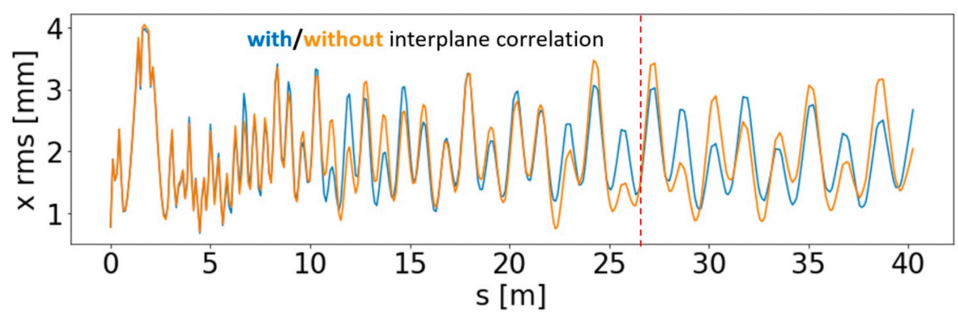

Figure 2: Comparison of horizontal beam size through PyORBIT simulation of SNS MEBT and DTL.

Figure 9: RMS beam size evolution for a correlated/decorrelated initial beam in the SNS linac. Presented at IPAC (2021).

I wanted to find out exactly how the 6D phase space correlations were affecting the beam dynamics, including halo formation. When I reproduced this figure, though, I noticed something strange. The rms bunch length (z) spiked halfway through the simulation.

Plotting the phase space coordinates at these locations made me realize that some particles were falling *way* behind the bunch. Eventually, these particles were intercepted by the transverse apertures and removed from the simulation. It doesn't make sense to keep these particles in the bunch, so I added energy and phase apertures throughout the lattice to remove particles as soon as they deviated from the synchronous coordinates. The rms bunch length was now

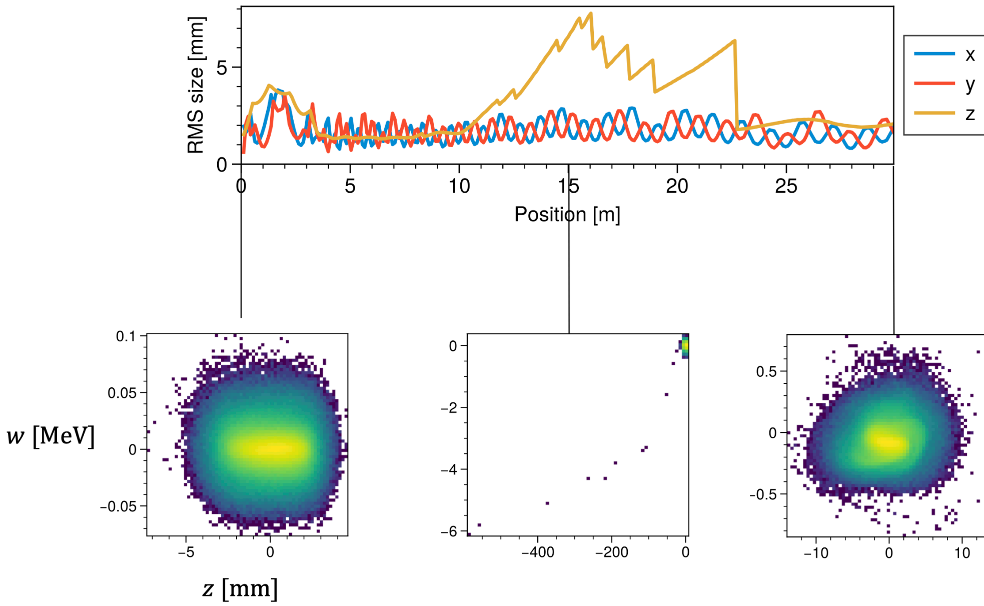

Figure 10: Some particles are lagging behind the bunch...

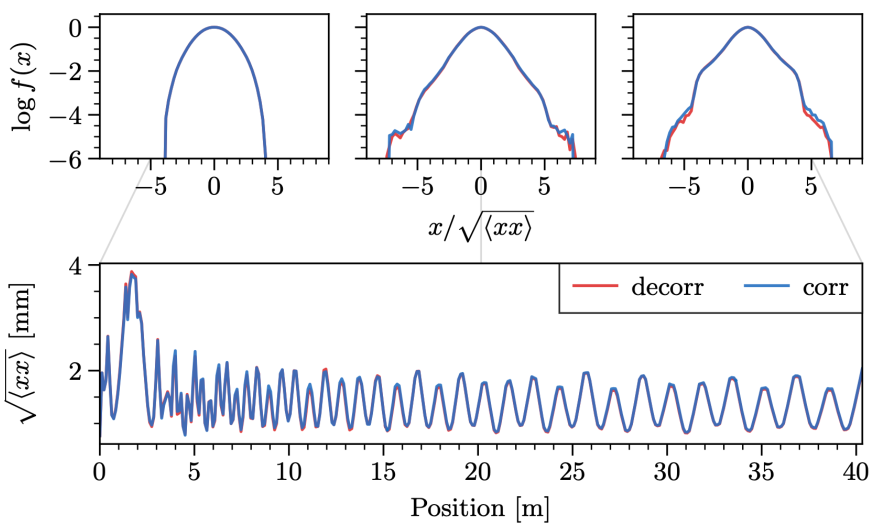

Figure 11: RMS beam sizes after adding longitudinal apertures. Compare to Figure 9.

well-behaved, but I no longer saw any difference between the transverse sizes of the correlated and decorrelated bunches.

What's going on? It turns out that the lost particles were affecting the space charge calculation. To compute the beam's electric field, we solve the Poisson equation on a grid:

$$\nabla \cdot \nabla \phi(x, y, z) = \frac{\rho(x, y, z)}{\epsilon_0}, \tag{4}$$

where ϕ is the electric potential and $ is the charge density. In PyORBIT, the grid expands to include all particles. In Figure 10, the grid would expand in the middle plot to include the z coordinates behind the bunch. This would leave almost all particles in one z bin, giving an inaccurate charge density and space charge forces.

So that's settled. But it also raises the question: do cross-plane correlations matter *at all*? Figure 11 shows that the one-dimensional beam density is independent of the initial cross-plane correlations, even at the level of beam halo. Thus the answer is no: according to our model, cross-plane correlations do not affect the beam dynamics in the SNS. The more detailed view in Figure 12 shows that the differences between the distributions disappear quickly, within a few meters. You can see the hollow initial z distribution in the 1D lineout compared to the peaked z distribution; this represents a correlation because the distribution is only hollow near $x = y = p_x = p_y = 0$. The lineouts merge soon after acceleration begins. The output distributions are *both* highly correlated by the end of the figure.

Conclusion

If these calculations are correct, and if our linac model is realistic, then these findings are significant. We suspect that measuring $f(x, p_x)$, $f(y, p_y)$, and $f(z, p_z)$ should give the same results as $f(x, p_x, y, p_y, z, p_z)$. Since 2D measurements are easy to measure, it gives hope to many existing accelerators. Any remaining discrepancies would be due to an inaccurate lattice model, not the initial beam. Of course, all of this needs experimental validation.

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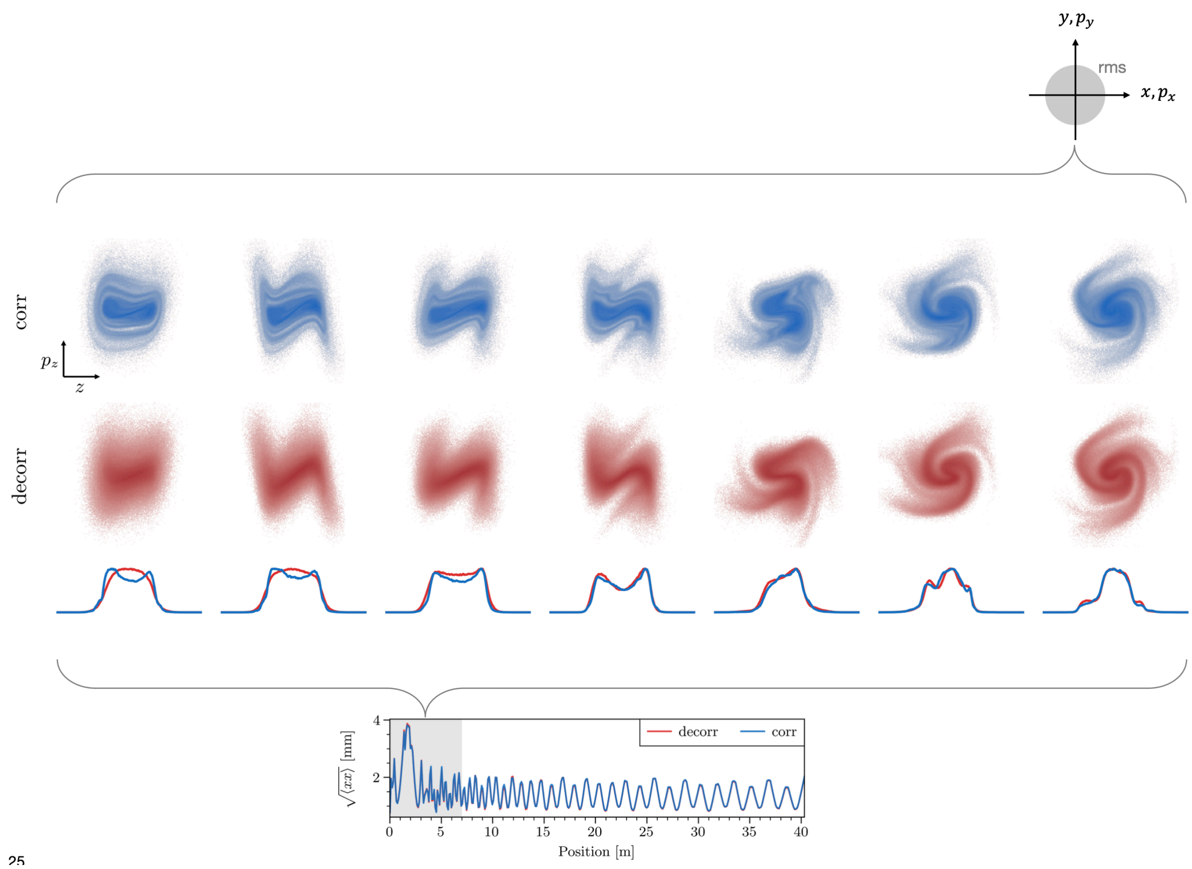

Figure 12: Longitudinal phase space evolution in the linac. Each plot is the longitudinal phase space (z-p_z) distribution within a 4D ball in the transverse plane. 1D lineouts onto the z axis are plotted on the bottom row. Blue = correlated, red = decorrelated initial bunch.

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