CHALLENGES IN BENCHMARKING OF SIMULATION CODES AGAINST REAL HIGH INTENSITY ACCELERATORS

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Abstract

Benchmarking of simulation codes for linear or circular accelerators involves several levels of complexity, which will be revisited and discussed in this talk. We first give some examples of how simulation codes have been validated towards the goal of gaining confidence about the underlying physics mechanisms. Besides such physics validation a bigger issue has been to feed codes with an accurate enough model of the real machine. We address these questions by discussing several examples of benchmarking efforts, their achievements as well as the limits and difficulties that have been encountered.

INTRODUCTION

Benchmarking of simulation codes for high-intensity linear accelerators or synchrotrons is necessary in order to raise confidence in predictions on beam loss and beam quality for new projects like the FAIR-project [1], C-ADS and C-SNS [2], ESS [3], IFMIF [4] and others; or to explain observations and possibly improve the performance of running high intensity machines in different laboratories (like SNS [5], J-PARC [6] or the CERN injectors into to LHC [7]). The main efforts of code validation in this field have started in the late 1990's with the coming of the SNS and at the same time the steadily increasing performance of computers.

A few remarks on the historical evolution in this field may be appropriate. The main step of development needed for high intensity accelerators simulation has been the particle-in-cell (PIC) technique. Actually PIC simulation was already developed in the 1960's primarily for fluid dynamics, plasma physics and magnetohydrodynamics. Already in the 1970's PIC codes were commonly used to model plasmas in all fusion laboratories around the world. Major challenges in this new approach have been short wavelength fluctuations in density and electromagnetic fields and the need to overcome limitations from unphysical fluctuations. Progress has been tremendous, and as of today the largest plasma or fluid PIC simulations are done with up to 10^{10} particles using as many as 10^5 processors.

In accelerator physics PIC codes came into practice with about 15 to 20 years of delay - mostly because there was no need. In the 1970's primarily single particle dynamics was used. Coulomb interaction was gradually introduced as binary interaction between particles, and limited to a few thousand simulation particles. In the 1980's the first PIC simulations were started in a number accelerator labs, partly driven by the idea of using accelerators as drivers for inertial fusion. A full transition to PIC codes occurred nearly everywhere in the late 1990's. Although intense beams have something in common with (un-neutralized) plasmas, the challenges in PIC simulation for accelerator beams have been very different from those of plasmas or fluids: internal collective effects are weak, and the main challenge is the interacting with the surrounding structure and the proper modelling of it.

THE BENCHMARKING "PROBLEM"

With the enormously grown capabilities in computer simulation expectations have grown to use these codes for reliable predictions and even for improvements of accelerators. It is often overlooked that codes can only be a simplified model of reality, but we have practically unlimited information about this model. The problem of the experiment, on the other hand, is a different one. The experiment is a perfect model, but information on the physics in it is always very limited due to diagnostics limitation. This makes it so difficult to bring the two approaches to some level of mutual agreement. The inherent dilemma in code benchmarking crystallizes in the following observation [8]: "No one believes the simulation results, except the one who performed the calculations, and everyone believes the experimental results, except the one who performed the experiment." Clearly, in most eyes the experimentalist has a strategic advantage as the real world stands behind him.

In order to overcome this difficulty it has been accepted that benchmarking of simulation should be seen on basically two levels not to be mixed up: code verification and code validation.

Code Verification

The task is to verify that a computer code represents the intended conceptual model: multi-particles with smoothed space charge forces, idealized magnets and cavities etc.. At this level codes can be compared with analytical models (important also for modelling of experiments) to verify the accuracy of a code with regard to an idealized model accelerator. The basic questions are "Is my code doing what it is written for? Is the algorithm programmed correctly? Is the grid resolution of my Poisson solver consistent with some criteria?"

Code Validation

The goal is to validate a code as sufficient to describe certain experiments - the emphasis is on "certain". Therefore it should not be claimed that the code is validated - it is only a particular calculation or application, which has been validated. Questions are: "Is my code good enough to make predictions for the real machine? Do I have the same

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closed orbit, same aperture limitations, a (sufficiently) accurate space charge calculation?" The focus of this paper will be on validation.

MAJOR LINAC BENCHMARKING EFFORTS

Every new project has evidenced the need for progress in linac code benchmarking. Most of the development occurred over the last decade, we therefore highlight below some of the achievements as well as open questions.

Early SNS Code Comparison

With the coming on the horizon of the first linac spallation neutron source (the SNS) the need for benchmarking linac design codes became obvious. Participating codes have been Parmila, Parmela, Partran, Impact and Linac. The first effort was based on a real design lattice and a well-matched initial distribution from the RFQ. Tracking through the first DTL tank with 10 transverse focusing periods showed excellent agreement in rms emittance behavior and typically $\pm 5\%$ deviations in the 99% emittances [9].

European HIPPI Code Validation

The European HIPPI (High Intensity Pulsed Proton Injector) Project [10] (2003-08) was a collaborative effort between several laboratories (CERN, CEA, GSI, FZJ, RAL, Frankfurt university) to strengthen the basis for future high intensity linacs like the CERN-SPL and the FAIR p injector. HIPPI helped "politicall" to justify a dedicated experimental campaign at the GSI-UNILAC, which was one of the important conditions for its success in benchmarking. The experiments concentrated on tank A1 of the UNILAC with 60 cells (10 transverse periods) and a variable transverse focusing as shown in Fig. 1. This "free knob" of the UNILAC (as accelerator for all ion masses), which allowed a variation of the transverse phase advance between 30^o and 100^o for Ar^{18+} turned out to be essential for the success of the campaign. As in most linacs a direct measurement of the initial distribution wasn't possible at UNILAC, and simple WB or Gaussian approximations were found insufficient. An analytical formula fitted to the data was found to give the best fit for the 6D phase space distribution including tails (details see Ref. [10]). This procedure required a transformation of the format of a distribution from DYNAMION simulation to the format of the measured data from the slit/grid measurement device (Fig. 2).

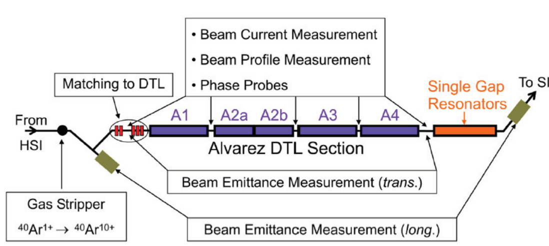

Figure 1: Schematic view of the experimental set-up around the first tank (A1) of the UNILAC DTL.

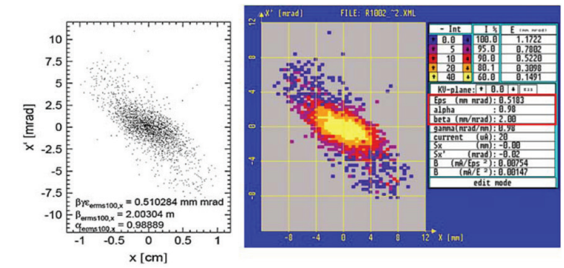

Figure 2: Transformation of format of a distribution from DYNAMION simulation (left) to the format of measured data (right) [10].

Figure 3 shows a comparison between experiment and simulation [11], using the Dynamion code [12], firstly with a "poor" initial matching, followed by an improved rematching. It is noted that obtaining results in terms of the phase advance (as free knob) is essential, as otherwise incidental agreement at some values of the phase advance could be very misleading.

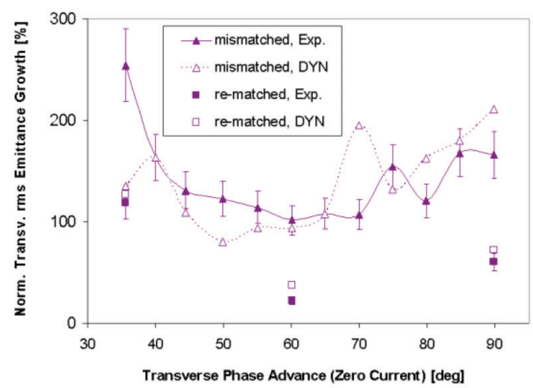

Figure 3: Relative growth of mean value of horizontal and vertical rms emittance at the end of the DTL as a function of zero current phase advance [11].

For mismatched beams the situation was quite different as shown in Fig. 4. Possible explanations for the discrepancies are: the gap modeling off-axis varies between codes; the space charge calculations far off-axis could be more sensitive; a more "chaotic" characteristic of beams for the non-periodic behavior in case of mismatch.

Validation of Space Charge Resonances in UNILAC

Two cases of successful code validation on the important issues of space charge resonances in the UNILAC have much benefitted from the preceding HIPPI campaigns and the learnings from it. It is important to include code validation of basic beam physics mechanisms into benchmarking to make sure that the underlying beam physics models are

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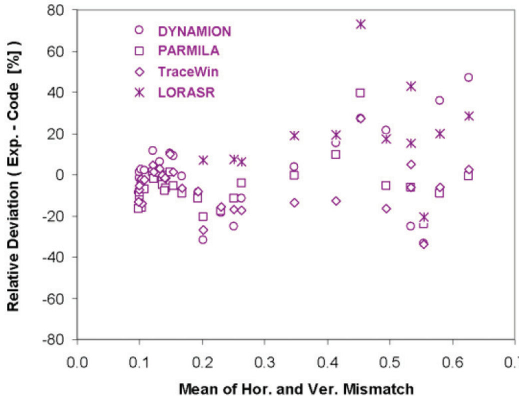

Figure 4: Relative deviation between final transverse rms emittances as measured and predicted by the codes versus the mean of horizontal and vertical mismatch to the DTL [11].

"robust" enough to be observable in real machines. At the same time these validations can demonstrate whether diagnostics is sufficient to extract the necessary information from an experiment.

The first experimental evidence of the 90^o stop-band in an RF linear accelerator was thus enabled at the UNILAC [13]. The simulations with Dynamion, Parmila and Tracewin gave convincing confirmation of the measurements and the existence of this stop-band as shown in Fig. 5. Actually, two stop-bands more or less coincide at

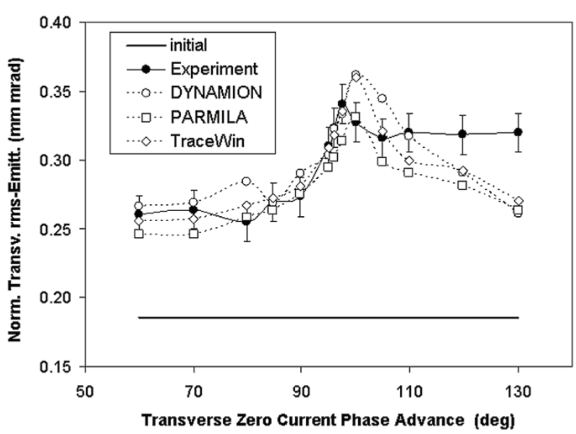

Figure 5: Mean of horizontal and vertical rms emittance as a function of the transverse zero current phase advance along the DTL [13].

90^o phase advance: the so-called envelope instability, and a fourth-order structure resonance. This experiment has given clear evidence that the stop-band is dominated by the fourth-order resonance, and not the envelope instability. This is shown in Fig. 6, where the four-fold structure is clearly visible in both, the slit-grid experimental data and the Dynamion simulation.

A related experiment confirmed the existence of reso-

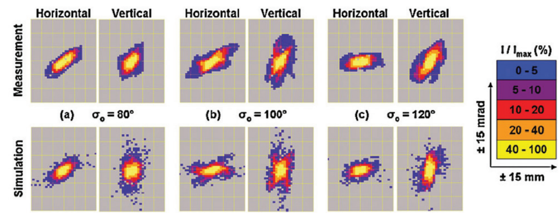

Figure 6: Upper row: measured phase space distributions at exit of DTL for different transverse zero current phase advances; Lower row: simulations.

nant exchange between the longitudinal and transverse rms emittances [14]. The initial ratio of these emittances is large - a factor 10 - at the UNILAC, and measurements showed a growth of transverse emittances at the condition of the "main resonance", where the ratio of longitudinal and transverse phase advances is near unity as shown in Fig. 7. In all cases the longitudinal zero current phase advance was constant at 43^o, with varied transverse phase advance. The measurements well validate the simulations, which have been obtained with the Dynamion and Tracewin codes.

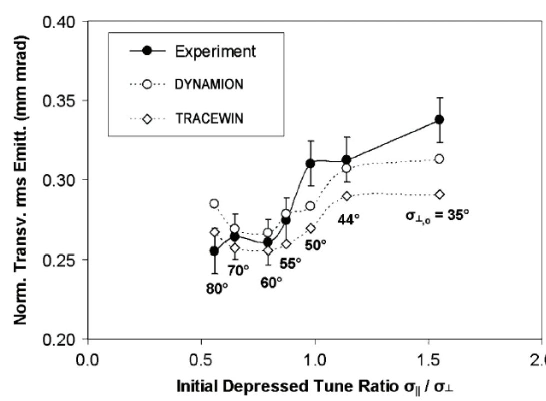

Figure 7: Measured stop-band for "main resonance" of emittance transfer in UNILAC [14].

Tune foot prints of the simulations for different values of the transverse phase advance can be plotted in stability charts for the emittance ratio 10 as shown in Fig. 8.

SNS Campaigns on Code Validation

Significant efforts to reconcile simulated and measured beam parameters have been made at the linear accelerator of the SNS and summarized at the preceding workshop [15]. As it is one of the newest and highest intensity proton linacs and advanced computer simulation tools were used during its design, furthermore it is equipped with a comprehensive set of beam diagnostics, these campaigns reflect the state-of-the-art in what is possible to reconcile code modelling and real machine measurement. At the same time they illustrate the kind of difficulty effective and convincing benchmarking is still facing; and the challenges

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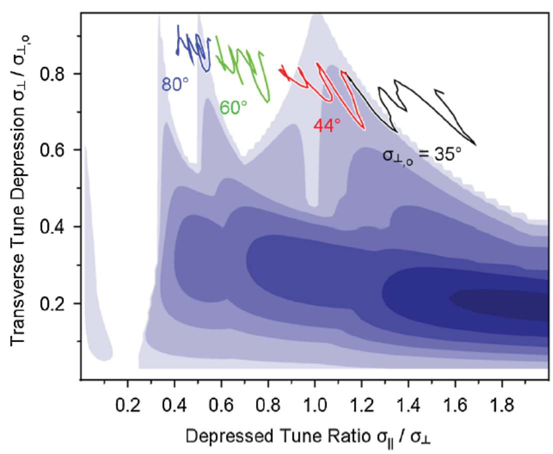

Figure 8: Stability chart for UNILAC with tune foot prints near the "main resonance", for different values of transverse phase advance.

that will have to be met in bridging the still large gap between codes and a complex real machine.

One of the learnings of the SNS campaigns has been that measurements and simulations often look similar visually. However, quantitative data from these measurements sometimes show large discrepancies with model calculations with the XAL-code [15]. This is illustrated by a comparison with the measured dependence of the rms emittance vs. the re-buncher RF phase as shown in Fig. 9, which shows significant disagreement.

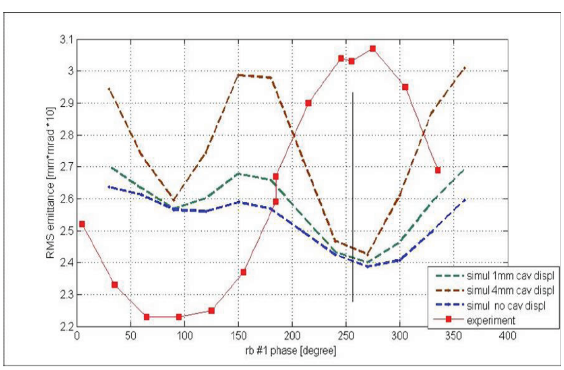

Figure 9: Measured (solid line) and simulated (dashed lines) dependence of the transverse rms emittance vs. re-buncher phase (courtesy of A. Alexandrov).

Similar findings have been obtained for measured and simulated (PARMILA) bunch length data in the SNS CCL as shown in Fig. 10 [15]. An attempt to fit the model to the measurements at three points was quite successful, but simultaneous fitting to four points appeared much more difficult. The beam size oscillations suggest a significant mismatch at the CCL entrance, which can be an important beam dynamics issue. Yet they are at the limit of the available diagnostics resolution and therefore require further study.

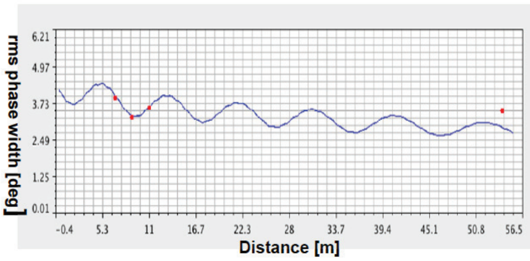

Figure 10: Comparison of the measured longitudinal rms bunch size (red dots) with the model (solid line) at four locations in the SNS CCL (courtesy of A. Alexandrov).

MAJOR RING BENCHMARKING EFFORTS

CERN-PS Experiments in 2002-2004

An important milestone in circular machine code validation was a series of high intensity measurements at the CERN Proton synchrotron in the years 2002-2004. A detailed benchmarking of simulation models with long-term (10^5 to 10^6 turns) effects at high intensity or high phase space density was seen crucial for the SIS100 of the FAIR project [1], where it is necessary to hold the high-intensity bunches between injections over typically 1 s at a loss level not exceeding typically 1%, likewise for the optimum performance of the CERN Proton Synchrotron for high-intensity beams. A major focus of these studies was the combined effect of space charge and nonlinear resonances and its impact on halo formation and/or beam loss.

The measurements were carried out as part of a high intensity machine development time at the PS in October 2002, and simulations were performed with the MICROMAP code employing a (non-selfconsistent) "frozen-in" space charge model [16]. The number of protons in the single bunch (200 ns long) was 10^{12}, and the maximum space charge tune shift was 0.12 vertically and 0.075 horizontally. One of the main difficulties was to reconcile the measured beam loss on the resonance, which was exceeding 30%, with the simulated one as shown in Fig. 11. An earlier big discrepancy (neglecting chromaticity in the simulation, green curve) could be partly overcome by including chromaticity in the simulations, which was an additional effect to space charge tune modulation and its possible impact on the issue of resonance trapping [17].

SIS 18 Validation of Nonlinear Resonances

The scope of the S317-campaign (2007-10) [18] was analogous to the earlier CERN-PS campaign to validate MICROMAP code modelling of a space charge driven nonlinear resonance crossing in an ion synchrotron, but this time with an external sextupole error. The new data extend the previous observations by a complete set of measurements comparing beams with and without rf, both at low and high intensity. The correlation between transverse beam loss and simultaneous bunch length shorten-

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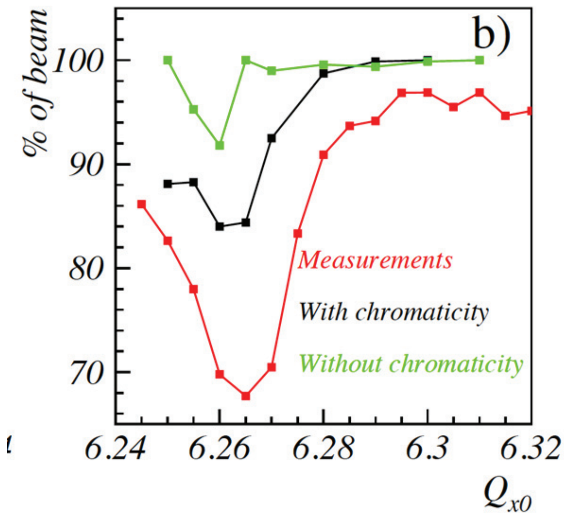

Figure 11: Beam loss prediction for the CERN PS-experiment: the black curve gives the updated simulation beam loss including chromaticity.

ing provides strong evidence that the measured emittance and the loss in intensity are indeed caused by periodic resonance crossing, leading to the main effect of scattering but also to a lesser extent to the trapping of particles due to the combined effect of the nonlinear resonance and the space charge. Therefore, in spite of the intrinsic differences between sextupole and octupole driven resonances, space charge leads to similar patterns in the beam response.

The comparison of the code predictions with the experimental results shown in Fig. 12 has given reasonably good agreement in spite of the limited knowledge of the SIS18 synchrotron lattice (closed orbit, multipole strengths etc), which does not allow a complete simulation of the real experimental conditions. Surprisingly, the simulation can only explain about 50% of the measured beam loss - similar to the results of Fig. 11. The issue of lack of self-consistency, which feeds back to the beam distribution, needs to be addressed in future studies.

SNS ORBIT Validation of Transverse Instability

The ability of the ORBIT code to model a transverse instability due to the kicker impedance was validated during a high intensity beam physics study in the SNS [19]. A transverse dipole instability in the vertical direction characterized by a frequency spectrum peaked at about 6 MHz was observed in the accumulator ring for a coasting beam stored for 10000 turns. From the observed 1036 turns growth time for n=12 (red line in Fig. 13) a kicker impedance of 28 kOhm/m was derived, which agrees well with the measured earlier 30 kOhm/m in the laboratory.

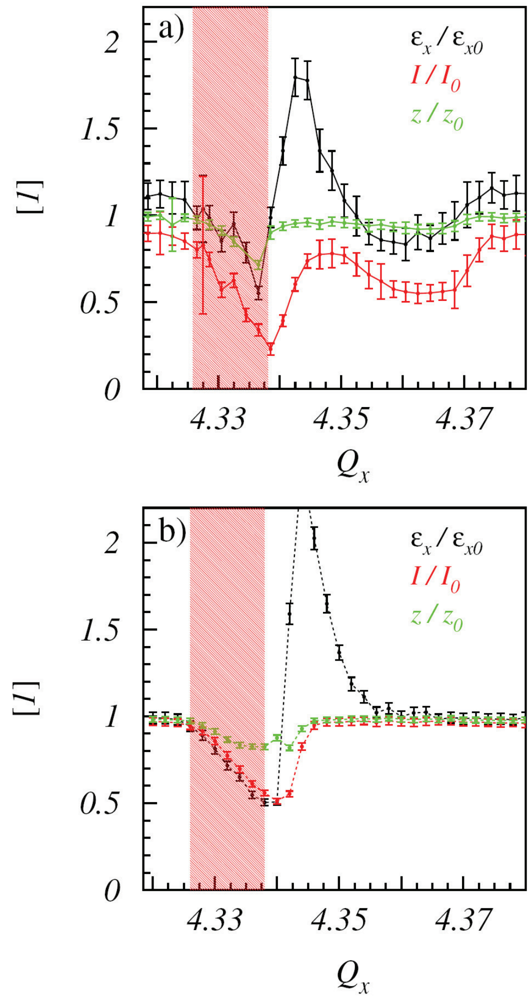

Figure 12: High intensity bunched beam: (a) Measured transverse-longitudinal beam response to the long-term storage as a function of the working points around the third order resonance. (b) Simulation of the same case.

Spectral Information and High Intensity - a Promising New Approach

First studies on possibly a new quality of code validation by using the spectral information due to a kicked head-tail mode have been recently carried out with the PATRIC code at GSI, in comparison with measured spectra from high intensity bunches in the SIS [20]. While for zero current the kicked bunch gives a periodic signal with the synchrotron period, high intensity leads to an entirely different spectrum, where the frequency of coupled modes (k=1,2,3 ...) is shifted by space charge (direct and image). Such a measured spectrum is shown in Fig. 14, with chromaticity corrected. Comparison with simulated spectra could allow direct validation of the code space charge model, which is hardly possible otherwise. With finite chromaticity and Landau damping present, some of the eigenmodes k are found - in simulation - to damp [21]. Thus the intrinsic distribution function (leading to Landau damping) would

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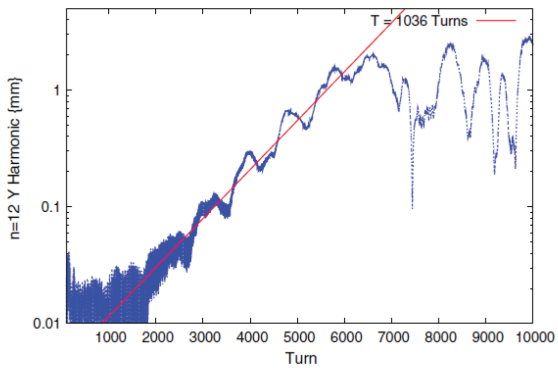

Figure 13: Vertical n=12 harmonic (in blue) versus turn number in the ORBIT extraction kicker instability simulation. The red line depicts an exponential growth time of 1036 turns (courtesy of J. Holmes).

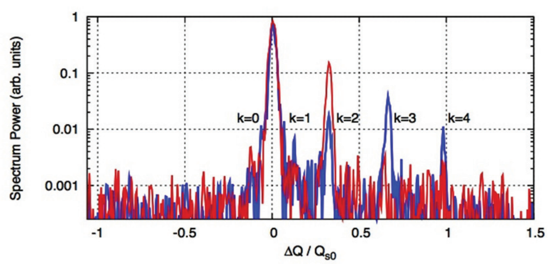

Figure 14: Measured spectrum of de-coherence of a kicked head-tail mode in the SIS at high intensity.

also leave an imprint on the spectrum. Due to the generally high accuracy of frequency measurements the spectral analysis of space charge (as well as impedance) and distribution function effects has a potential of becoming a promising tool in the future.

CONCLUDING REMARKS

Progress has been remarkable in a number of points, like successful validation of beam physics mechanisms, both for linacs and rings. It appears that quality standards of codes - especially in dealing with space charge - are generally high enough. Examples presented here also show that real validation requires a "free knob" and some variation of it to make sure that good agreement is not accidental. However, the "big" steps in code validation for high intensity accelerators still lie ahead. Comparison of simulation data with data from real accelerators is progressing slowly due to the challenges in dealing with limited diagnostics and the difficulties in importing the real accelerator model into a code. These problems are common to both, linac and ring benchmarking. In linac code validation the often poor agreement among codes and between codes and experiments for mismatched beams needs to be understood. The expectations to code developers, diagnostics people and to machine developers are higher than ever when looking at the desirable long-term goal of benchmarking: improvement and optimization of real machines. The direction is quite clear, but there is still a good piece of the way to go!

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