Challenges in Benchmarking of Simulation Codes against real High Intensity Accelerators

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Overview

- What is benchmarking?
  - Verification - Validation
- Major linac benchmarking campaigns of ~ last decade
  - enhanced confidence in codes
  - limitations - challenges
- Ring benchmarking campaigns
  - gaps between codes and machines
  - challenges for future steps
- Some conclusions

Brief history of Particle-in-Cell Codes

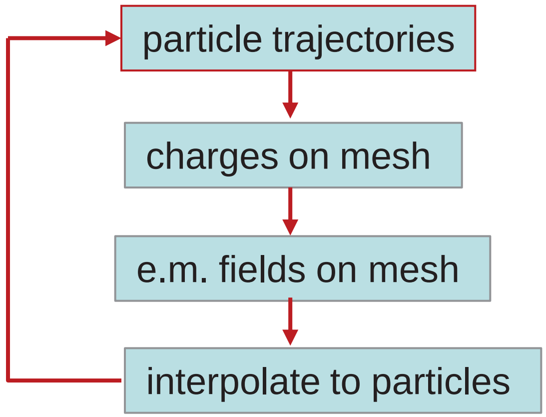
primary technique used in high intensity accelerators

Particle-in-Cell (PIC) Development

- > 1960's developed for **fluid dynamics, plasma physics, magneto-hydrodynamics** (Buneman, Dawson, Hockney, Birdsall, Morse and others)
- > 1970's common in **fusion laboratories**
- **challenges have been short-wavelength fluctuations in density and e.m. fields - scale lengths >> Debye screening length**
- today largest PIC 10^{10} particles 10^5 processors

PIC in Accelerators – 15-20 years delay

- > 1970's single particle dynamics
- binary Coulomb interaction starting
- ~1980 first PIC started in some labs
- in 1990's transition to PIC nearly everywhere
- **Challenges quite different from fluid or plasma PIC – bunch size: a < or ~ Debye screening length ($\lambda_D/a \sim k/k_0$ for $k/k_0 \ll 1$)**
- other methods disappearing or only for very special situations
  - o binary interaction – crystalline beams (some linac codes like DYNAMION)
  - o direct Vlasov solvers (1D or 2D)
  - o ...
- Benchmarking challenge started late 1990's with SNS ...



PIC advantage:
→ calculation time ~ N logN instead of N^2 (for binary interactions)

"Code Benchmarking" – a widespread problem

The benchmarking dilemma:

(from M. Greenwald, MIT, Computational Plasma Physics, 2004):

1. No one believes the simulation results, except the one who performed the calculations.

2. Everyone believes the experimental results, except the one who performed the experiment.

→ Experimentalist has a strategic advantage as real world stands behind him – really?

Levels of comparison

Code Development – Verification:

verify** that your computer code represents **the intended conceptual model

- *multi-particles with smoothed space charge force, idealized magnets + cavities*
- *compare with analytical models (important also for modeling of experiments)*
- *verify accuracy of code in idealized model accelerator*

↓

Experiments - Validation:

validate** that your code is **sufficient** to describe **certain experiments

- *never claim **the code** is validated - only **a particular calculation** or application*
- *think of **hardware and diagnostics** uncertainties*
- *good collaboration between theorist and experimentalist!*

↓

Reality:

only partly accessible – with uncertainties

- *no 6D phase space reconstruction, only projections*
- *...*

Examples

- Verification: "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?
  - ✓ ...
- Validation: "Is my code good enough to make predictions for the real machine?"
  - ✓ Do I have the same closed orbit?
  - ✓ Same aperture limitations?
  - ✓ Self-consistent space charge (rings)?
  - ✓ ...

Focus of this talk is on Validation!

Main questions

1. What is needed to bring my simulation model close to the real accelerator?
   - large number of parameters, partly unknown
   - do we have the right codes?
   - accuracy/completeness of diagnostics
2. Can we expect simulation to help towards optimizing machine performance?

❖ Still quite incomplete understanding of many issues

❖ many different personal views exist

❖ I apologize for material I have overlooked!

Overview on "dedicated" high intensity benchmarking efforts

Major campaigns of last decade

(elaborate experimental efforts and one/several codes)

Code comparison (Verification):

- ❑**SNS (>1999):** *S. Nath et al., Comparison of linac simulation codes, PAC01*

Validation with experiments:

- ❑**CERN-Proton Synchrotron with GSI (2002-04): MICROMAP Code + others**
- ❑**European HIPPI (High Intensity Pulsed Proton Injector) project (2003-08)**: verification **and** validation - several codes
- ❑**GSI (for FAIR high intensity upgrade) (>2009):** UNILAC + Codes
- ❑**SNS (2006→):** Orbit, Parmila
- ❑**Ring campaigns:**
  - ❑ **GSI-SIS18** (2007→)
  - ❑ **SNS (2006→)**: Orbit
- ❑CERN (2012 →): new campaign has been started for LHC
- ❑Expect J- PARC will be contributing significantly to this field

"Early" example: SNS benchmarking of linac codes (>1999)
limited to rms matched beams!

S. Nath et al., Comparison of linac simulation codes (SNS), PAC01
- using **well-matched initial distribution from RFQ**
- DTL 1st tank β=0.07-0.125
- 10 transverse focusing periods
- **excellent agreement in rms emittance growth**
- **deviations in "halo region" at 5-7 σ (beam loss predictions!)**

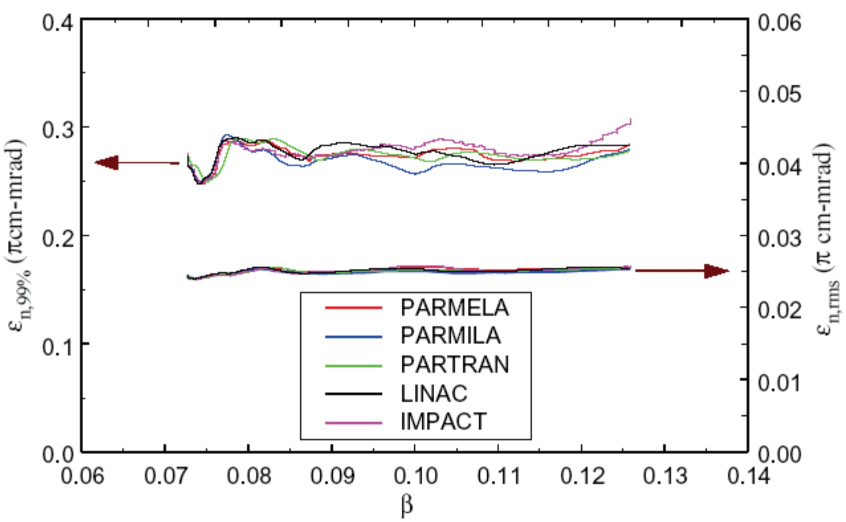


Figure 1. Transverse RMS and 99% emittance profiles through tank 1 of the DTL.

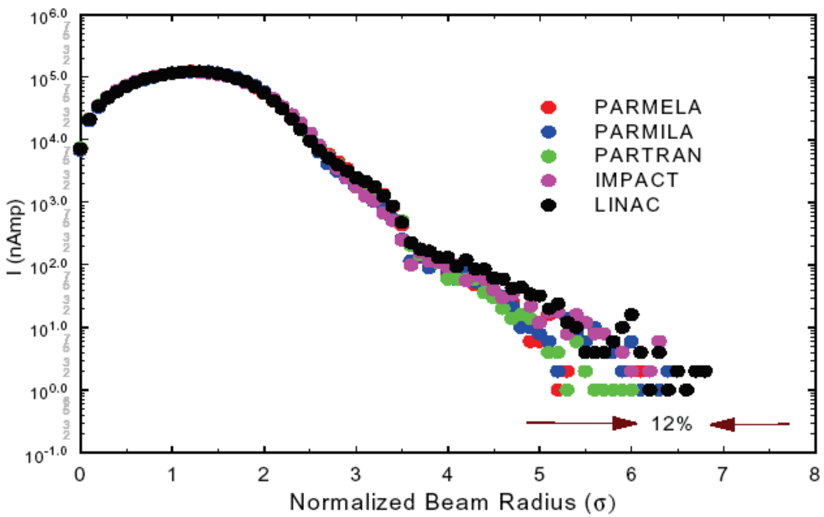


Figure 3. Simulated radial distribution at the output with different codes.

European HIPPI Project (2003-08)

(High Intensity Pulsed Proton Injector)

Strengthen basis for future high intensity linacs (CERN-SPL, FAIR p injector...)

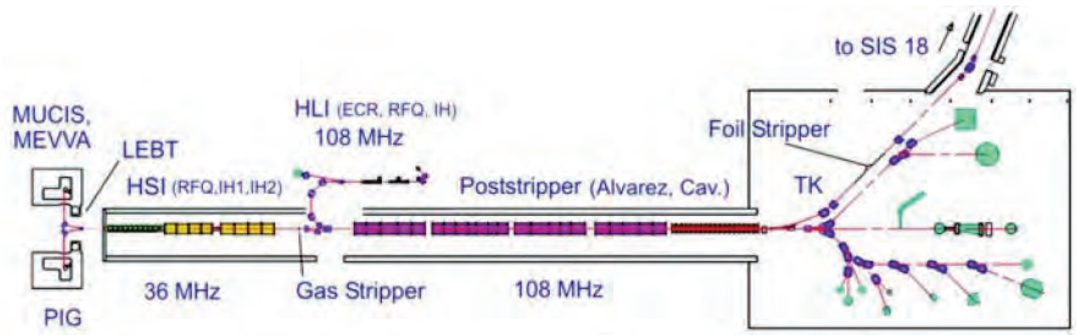


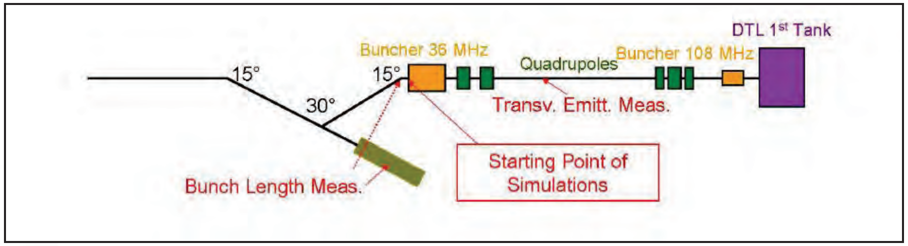
FIG. 1. (Color) The UNIversal Linear ACcelerator UNILAC at GSI.

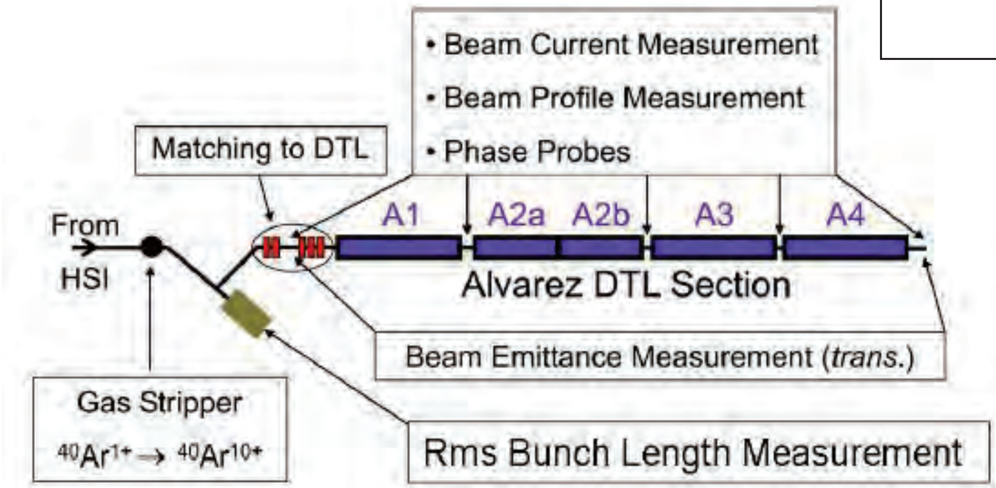
- EU supported partnership between CERN, CEA, GSI, FZJ, RAL, Frankfurt
- **HIPPI** helped "politically" to justify a real experimental campaign at GSI-UNILAC -
  - dedicated experiment - beyond mere machine development - most important condition for its success in benchmarking!
- UNILAC: DTL: 190 cells (~30 betatron periods A1... A4)
- A1: 60 cells (~10 transverse periods)
- variable transverse focusing for p → Uranium
- → "free knob": transverse phase advance could be varied from 30^0 ... 100^0 for Ar^{18+}

HIPPI cont'd

Benchmarking of measurement and simulation of transverse rms-emittance growth
L. Groening et al., PRST-AB 2008

- tedious reconstruction of initial 6D phase space distribution
- compared "well-matched" with mismatched beams





HIPPI cont'd

Good agreement for matched beams – poor for mismatched

Experiment – DYNAMION code

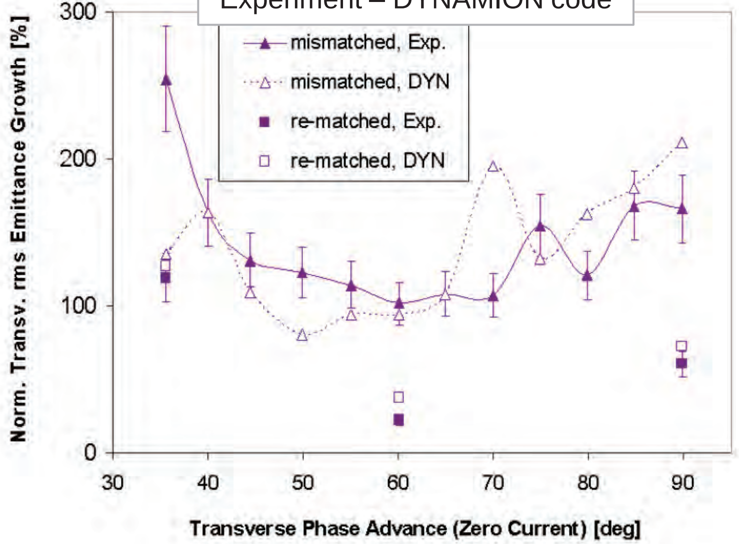


Figure 9: Relative growth of mean value of horizontal and vertical rms emittance at the end of the DTL as a function of σ_o. Data are shown for moderate mismatch and for the case of minimized mismatch.

code-experiment comparison for mismatched beam

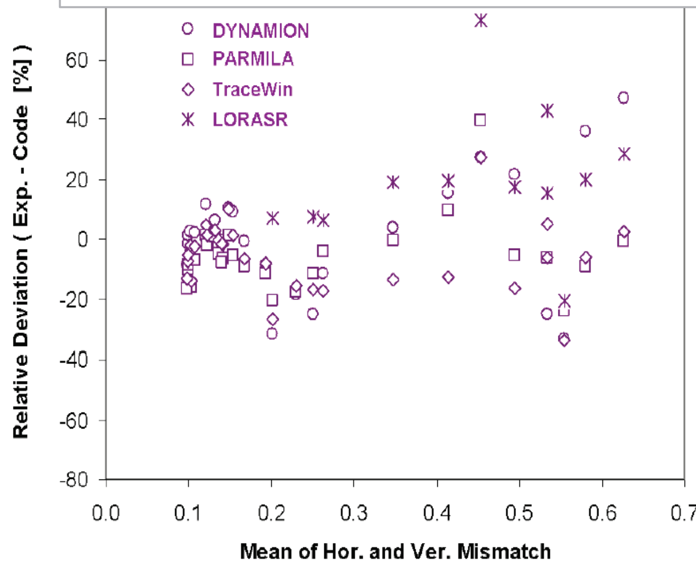


Figure 10: Relative deviation between final transverse rms emittances as measured and predicted by the codes versus the mean of horizontal and vertical mismatch to the DTL.

Possible explanations for mismatched beam discrepancies:

1. Gap modeling off-axis varies between codes
2. Space charge calculations far off-axis more sensitive?
3. More "chaotic" behavior for non-periodic system

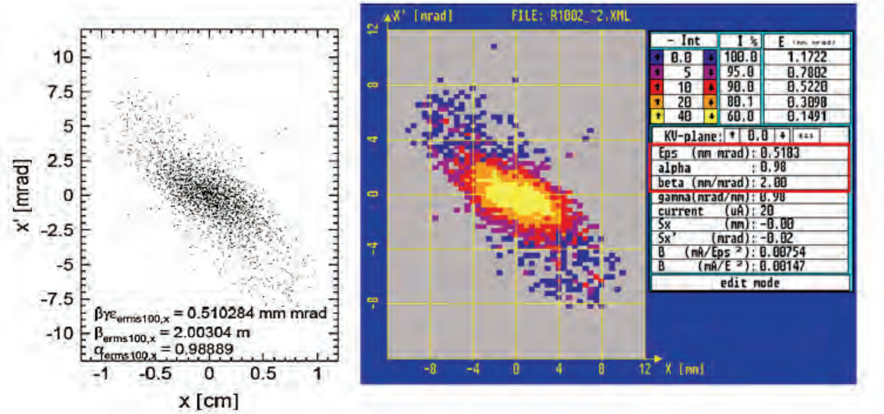
Initial distribution re-construction
- a major challenge *(L. Groening et al., PRSTAB-2008)*

- Real direct measurement at UNILAC injection wasn't possible
- Simple WB or Gaussian approximations not enough
- Analytical formula fitted to data – different powers in X and Y gave best fit for tails

$$\tilde{R}^2 = X^2 + X'^2 + Y^{1.2} + Y'^{1.2} + \Phi^2 + (\delta P/P)^2$$

$$f(\tilde{R}) = \frac{a}{2.5 \cdot 10^{-4} + \tilde{R}^{10}}, \quad \tilde{R} \le 1$$

$$f(\tilde{R}) = 0, \quad \tilde{R} > 1,$$



Transformation of format of a distribution from DYNAMION simulation (left) to the format of measured data (right) coming from slit/grid measurement device.
Normalized 100%-rms-Twiss parameters are highlighted in red.
→ Data reduction of simulation identical to measurement

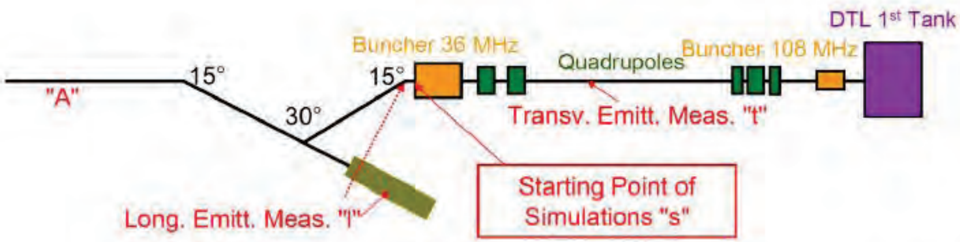


FIG. 6. (Color) Reference points used for reconstruction of the initial phase space distribution as needed for the simulations.

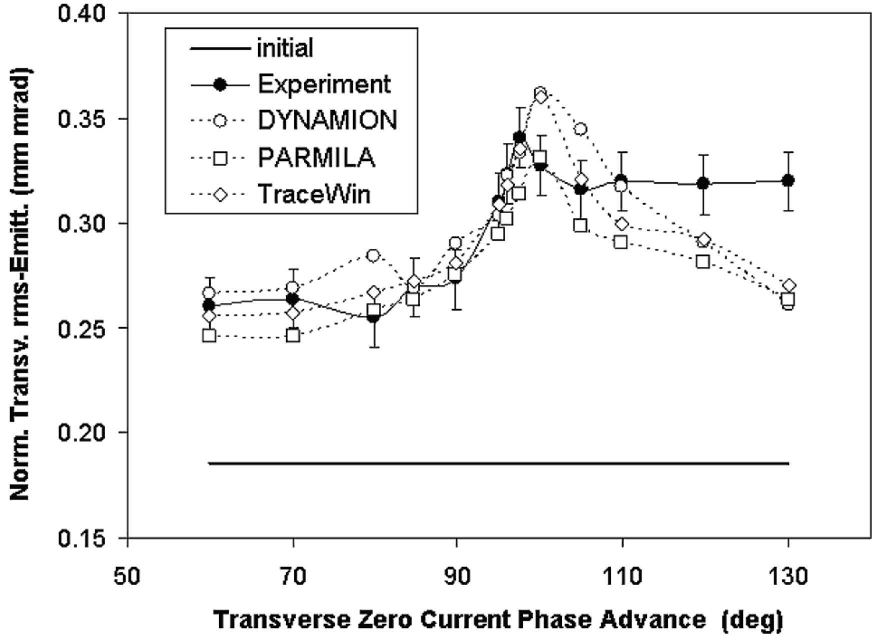
GSI-UNILAC: further code validation

using two "theoretical" concepts (2009)

- benefitted from HIPPI benchmarking campaign -

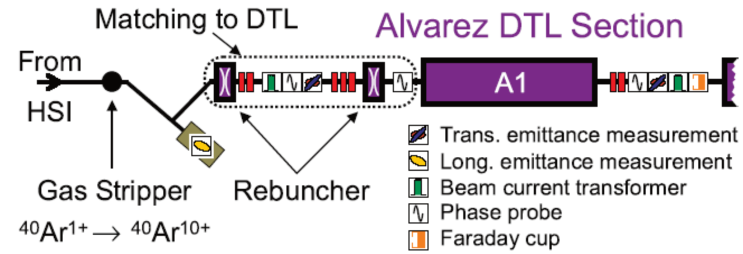
1. **"Experimental Evidence of the 90° Stop-Band in the GSI UNILAC"** L. Groening et al. PRL 102 (2009)
   - Resonance at $\sigma_{ox} > 90^0$ ($\sigma_x \sim 90^0$)
   - first experimental evidence in linac
2. **"Resonant exchange of longitudinal and transverse emittance at the UNILAC"** L. Groening et al. PRL 103 (2009)
   - first experimental evidence of emittance exchange
   - an issue for FAIR (highest current Uranium)

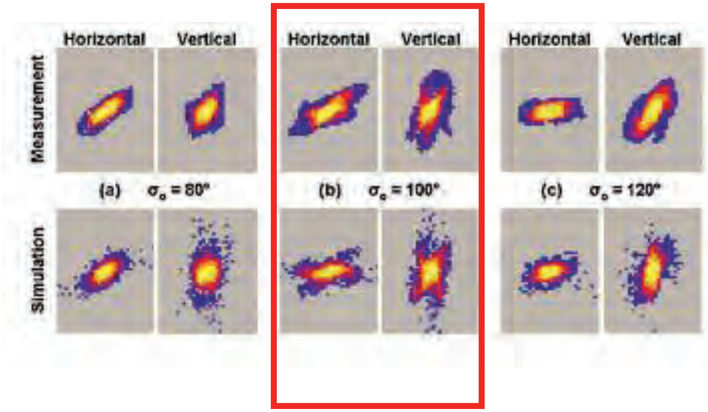
Case 1: $\sigma_{ox} > 90^0$ resonance measured at UNILAC (PRL, 2009)
- a successful code validation experiment



codes:

- DYNAMION: L. Groening
- PARMILA : D. Jeon
- TRACEWIN: D. Uriot





Clear evidence that fourth order resonance ($4\sigma \sim 360^0$) and not (competing) envelope instability

Case 2: Emittance exchange in UNILAC (PRL, 2009)

- first benchmarking of linac stability charts

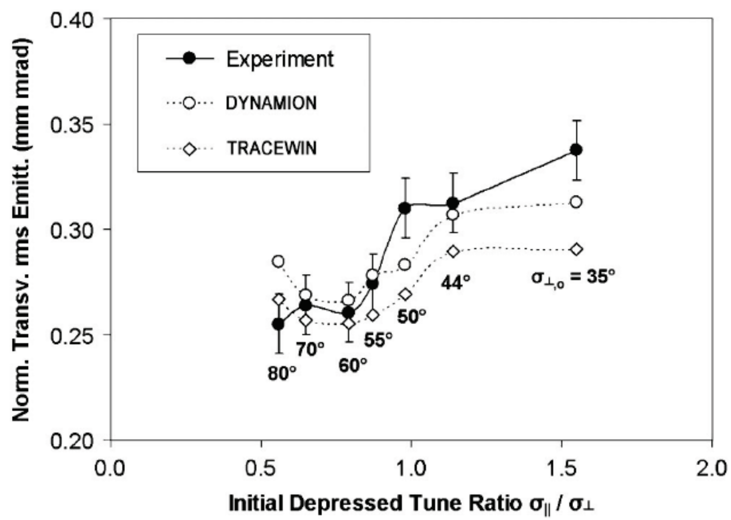
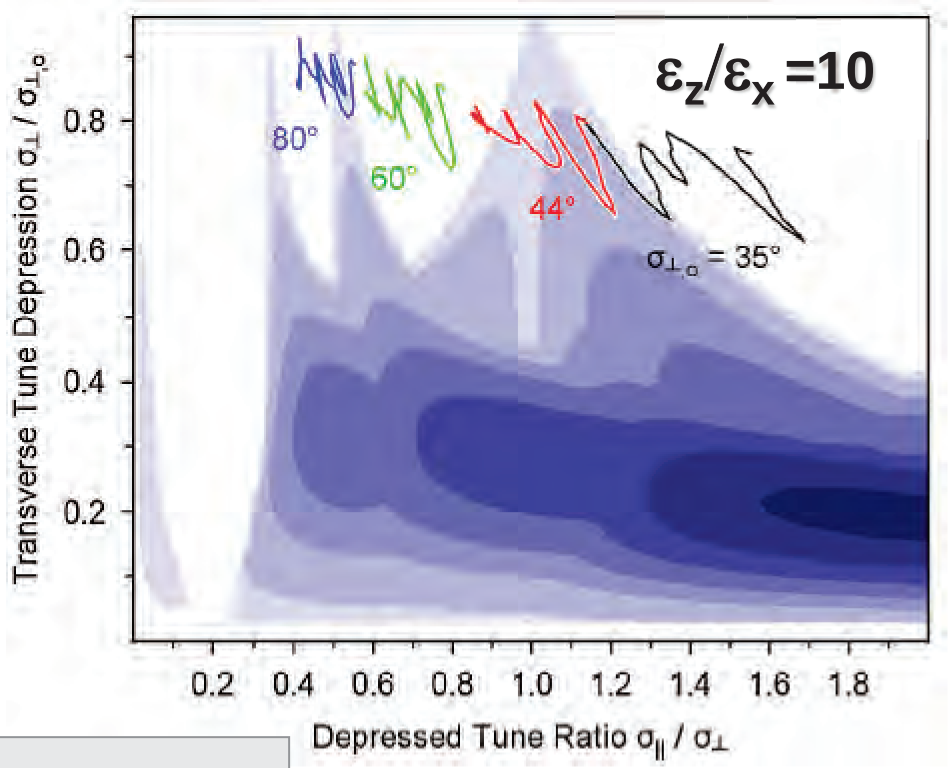


FIG. 4. Mean of horizontal and vertical rms emittance at the DTL exit as a function of the initial ratio of depressed longitudinal and transverse tune $\eta = \sigma_{\|}/\sigma_{\perp}$.



- far from equipartition
- driven by large energy anisotropy $\varepsilon_{lo}\sigma_{lo} \sim 10\ \varepsilon_{tr}\sigma_{tr}$
- observed in transverse plane (growth)
- an issue for future full intensity of U^{28+}

SNS –Linac campaigns (2010):

reconcile calculated and measured beam parameters?

- SNS one of best known high intensity machines -

source: A. Alexandrov, Challenges of reconciling theoretical and measured beam parameters at SNS, HB2010

Qualitative agreement:

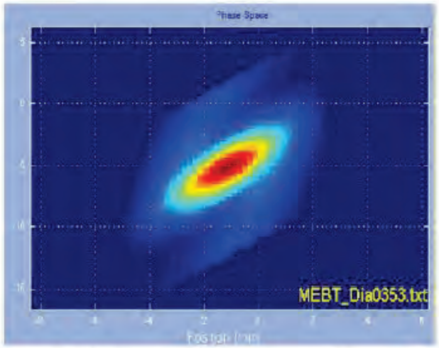


Figure 5a: Measured transverse emittance in the MEBT.

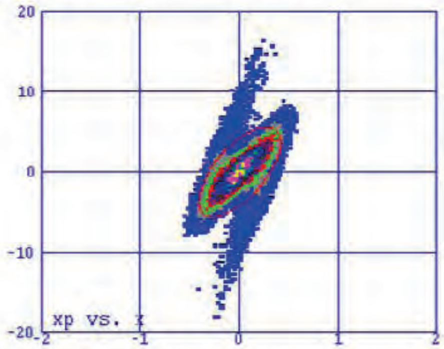


Figure 5b: Simulated transverse emittance in the MEBT.

However:

- big deviation in a series with rebuncher rf phase varied
- reveales quantitative behaviour

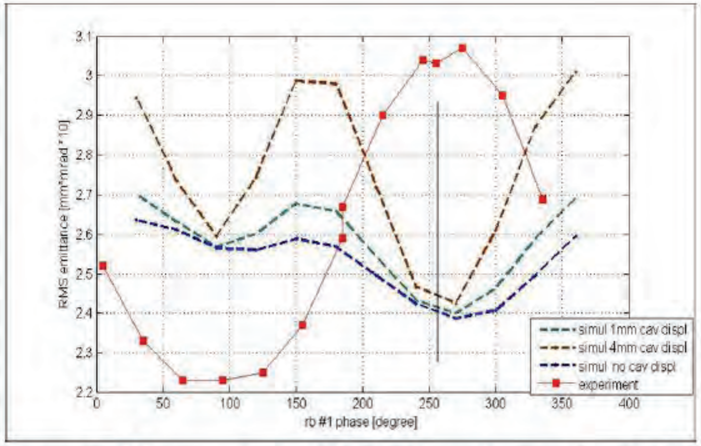


Figure 6: Measured (solid line) and simulated (dashed lines) dependence of the transverse rms emittance vs. the re-buncher phase.

cont'd SNS –Linac

Longitudinal rms bunch size - comparison of measurement and code model (*A. Alexandrov, 2010*):

- Three measured points well reproduced by model
- Fitting at four locations increasingly accurate
- Mismatch at entrance to CCL?

Conclusions:

- Significant uncertainty on real parameters of accelerators (more diagnostics)
- Minimize difference model-data by varying (many!) parameters
- **Challenge to (new) codes and diagnostics!**
- **This questions that "trend" to higher .e.m. field resolutions and larger N is useful!**

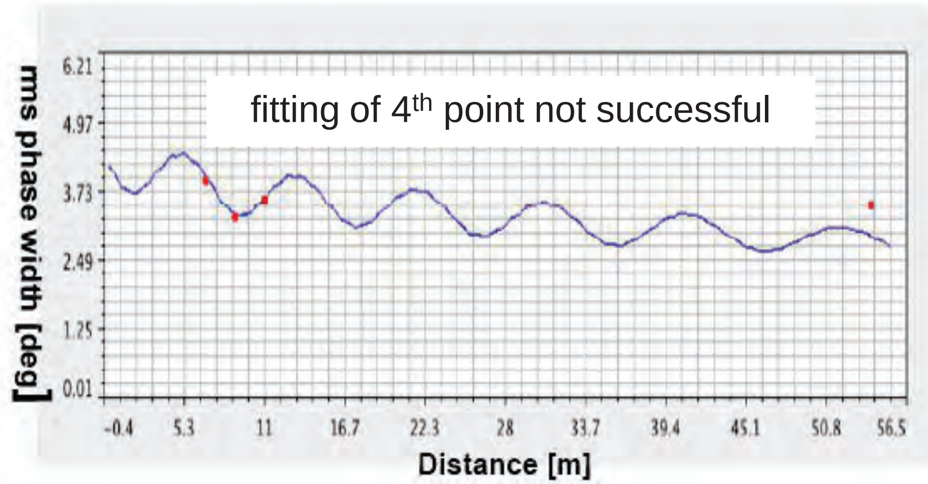


Figure 8: Comparison of the measured longitudinal rms bunch size (dots) with the model (solid line) at four locations in the SNS CCL.

Table 1 Beam Modeling Accuracy in the SNS Linac

	Transv. centroid	Transv. RMS	Long. centroid	Long. RMS
RFQ	NA	NA	NA	NA
MEBT	good	good	not so good	good
DTL	good	not so good	very good	NA
CCL	very good	not so good	very good	not so good
SCL	not so good	not so good	very good	NA

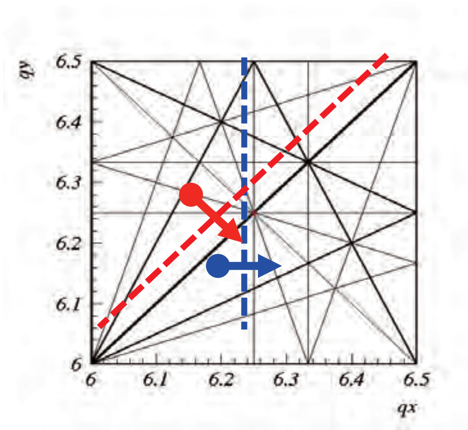
Ring codes benchmarking
CERN "space charge" campaigns 2002/04

long-term (~ second) real time

Carried out at CERN Proton Synchrotron

(M. Giovannozzi, M. Martini, E. Metral, G. Franchetti and I. Hofmann, PRSTAB 2003)

1. 2002: Octupole crossing resonance ($4Q_h=25$)
   1. controllable nonlinearity
   2. beam loss underestimated
   3. uncertainties on lattice – dynamic aperture!!!
2. 2003/04: Montague resonance ($2Q_h=2Q_v$)
   1. good starting point: intrinsic, less subject to particular machine, 3D aspects (very slow crossing) only recently resolved
   2. code comparisons
3. Importance of controlled "series definition"



CERN-Proton Synchrotron Benchmarking

Controlled octupole strength + space charge

Emittance comparison (2002) over 5x10^5 turns ("frozen" space charge):

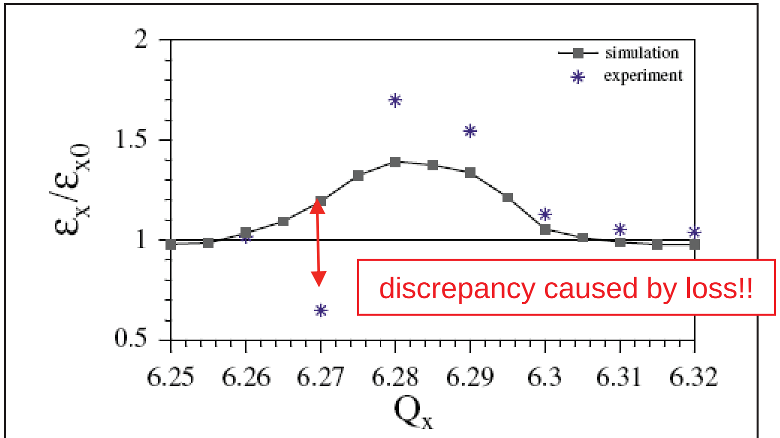
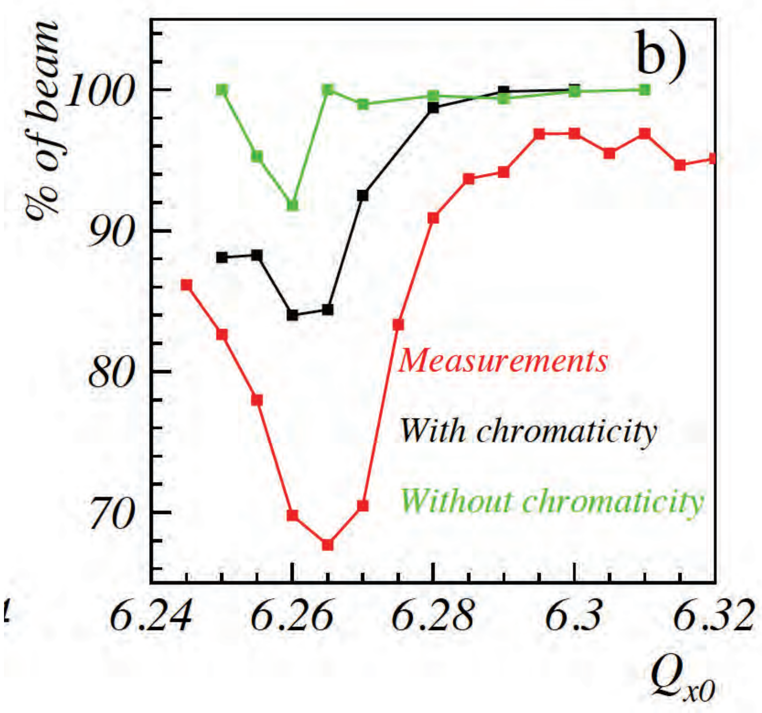


FIG. 5. (Color) 3D simulation using analytical space charge (40 A octupole). Shown are simulated rms emittances (Gaussian fit) after 5×10^5 turns and experimental values.

Intensity comparison updated later (2006):

- by including the chromaticity beam loss matched better
- still by factor 2 underestimated
- remaining uncertainties?

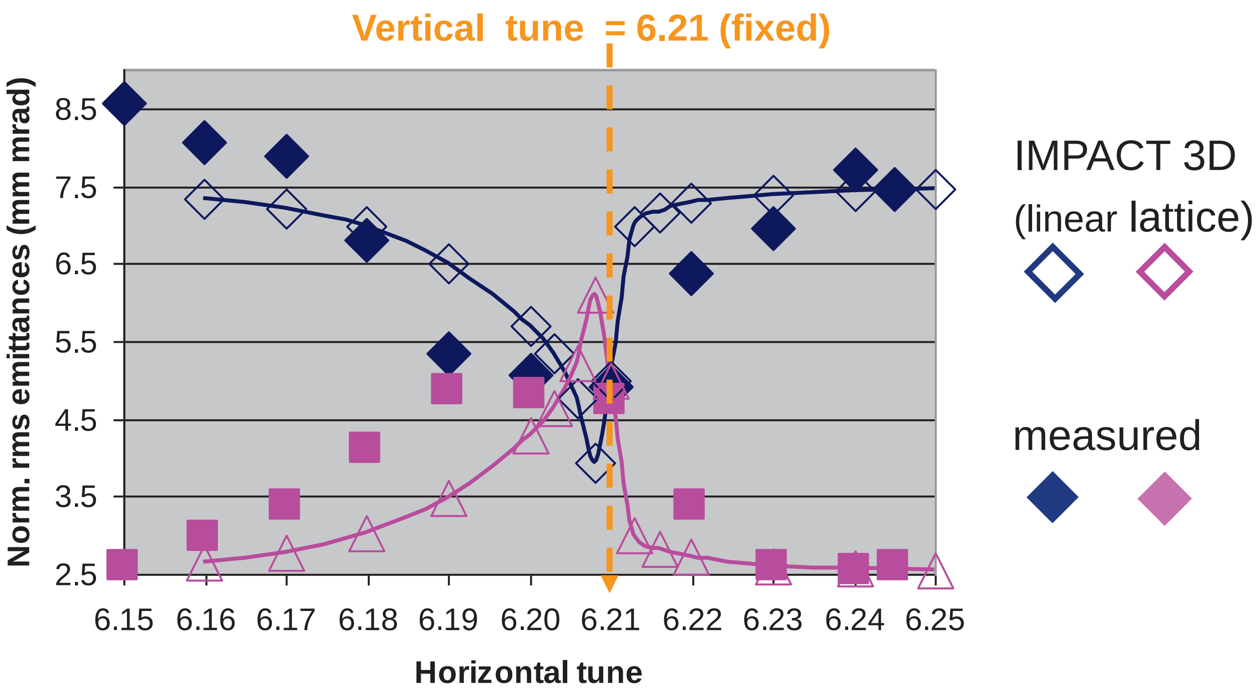


G. Franchetti and I. Hofmann, HB2006

CERN-PS: Montague emittance coupling resonance

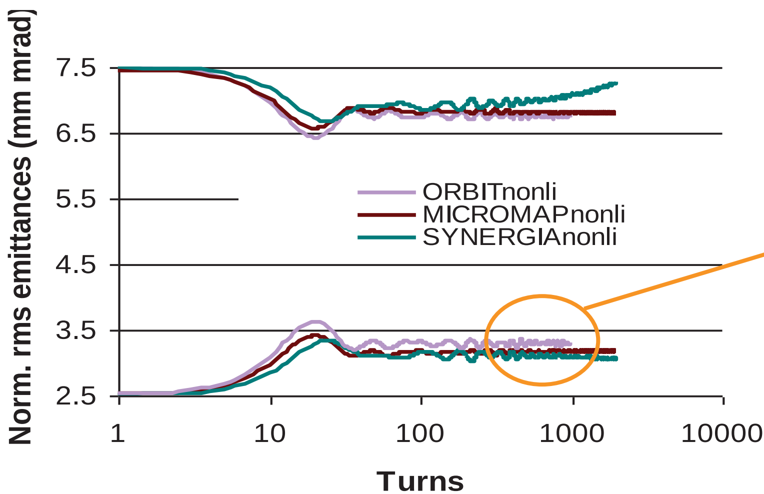
($\varepsilon_h = 3 \times \varepsilon_v$; $Q_h \rightarrow Q_v$)

- 2003: Issue for choice of ideal high-intensity working points
- Intrinsic space charge issue – largely "lattice independent"
- → quite good agreement (*E. Metral et al., HB2004)*



Used for "coasting beam" code benchmarking (2004) in realm of space charge and < 1000 turns

some discrepancies (*from nonlinear lattice?)* over 10^3 turns!



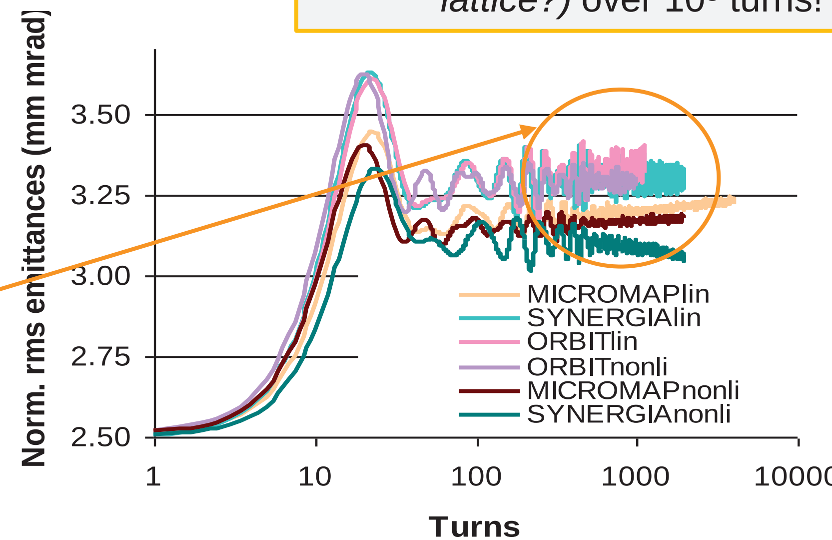
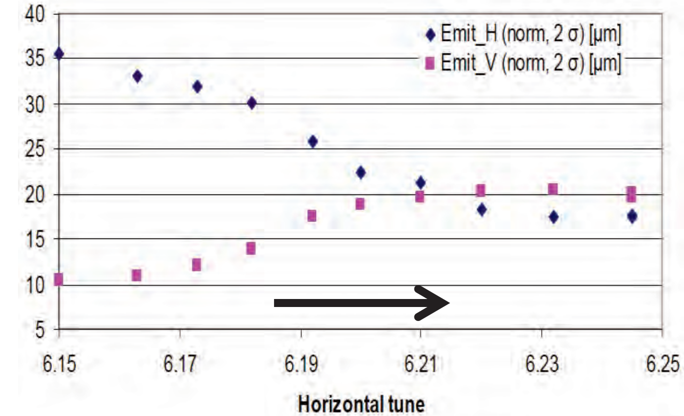


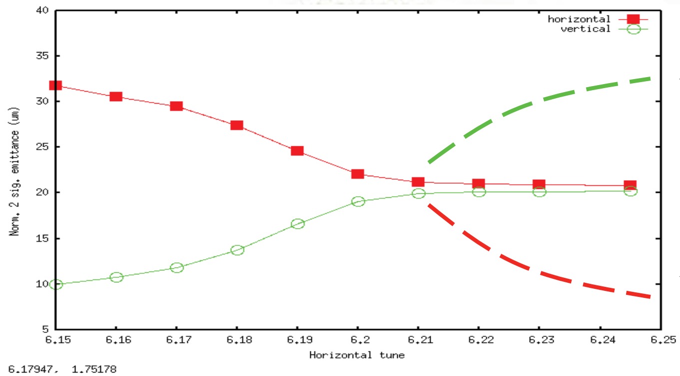
Table 1: Participating codes

Code	Lab	Dim	N
ACCSIM (ACC)	TRIUMF	$2\frac{1}{2}$ D	10^6
IMPACT (IMP)	LBNL	3D	10^6
MICROMAP (MIC)	GSI	2D	5×10^4
ORBIT (ORB)	ORNL	$2\frac{1}{2}$ D	10^6
SIMBAD (SIMB)	BNL	$2\frac{1}{2} D$	10^5
SIMPSONS (SIMP)	KEK	$2\frac{1}{2}$ D	10^4
SYNERGIA (SYN)	FNAL	3D	10^6

Recent update with fully self-consistent 3D long-term simulation for CERN-PS Montague study
(Ji Qiang et al., IPAC2012)

Dynamic crossing of stop-band:





IMPACT fully selfconsistent (3D space charge)

- 100.000 macropartices
- 65x65x129 grid points
- 50.000 turns
- nonlinear PS lattice

Slow synchrotron motion de-coheres correlation in 4D phase space
→ **new quality of benchmarking in rings**

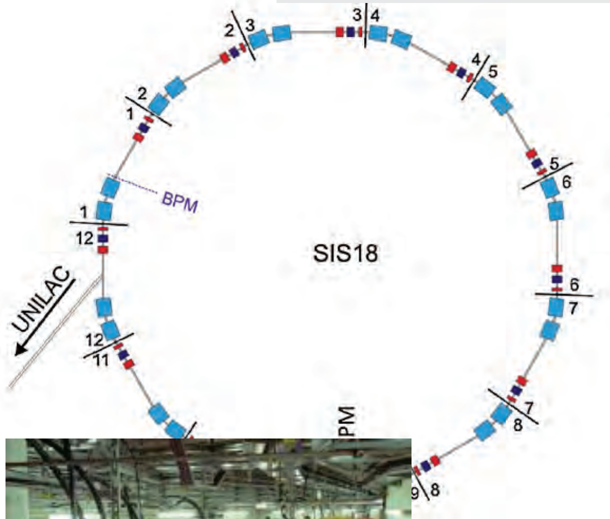
frozen synchrotron motion
- no mixing (decoherence) -

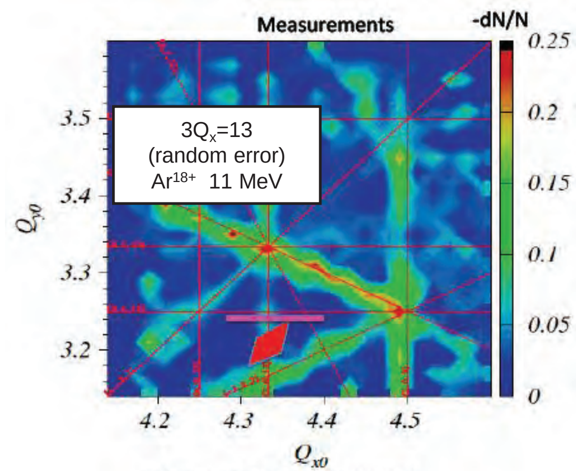
GSI

SIS 18 nonlinear resonance study (2007-10)

Expectation: Sufficient basis to predict beam loss in SIS100 of FAIR?

Dedicated experimental campaign SIS317 using random sextupole errors
G. Franchetti et al., PR-STAB 13 (2010)

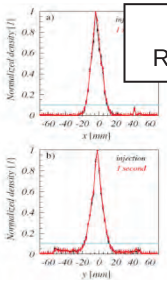




G. Franchetti et al., GSI-Acc-Note-2005-02-001

Application in FAIR:

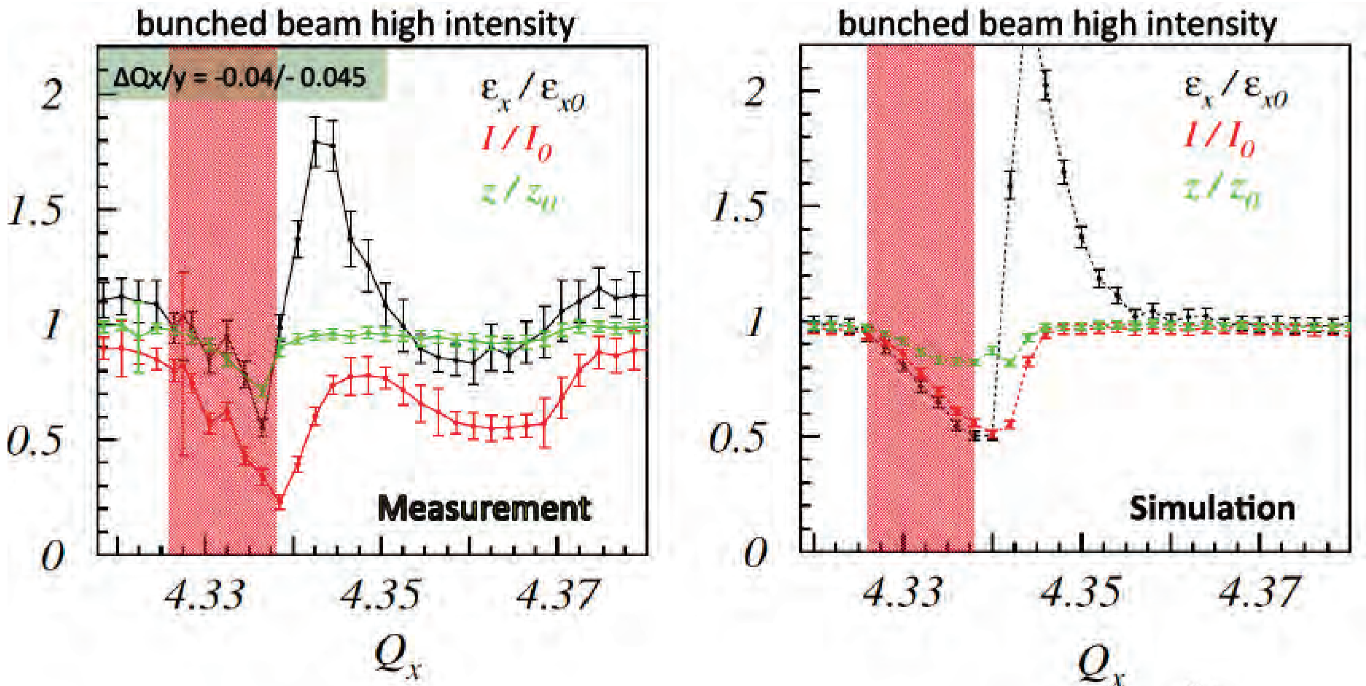
→ bunch into bucket transfer of SIS 100
- 1 sec holding
- ~ few % loss



emittance evolution:
RGM – non-destructive

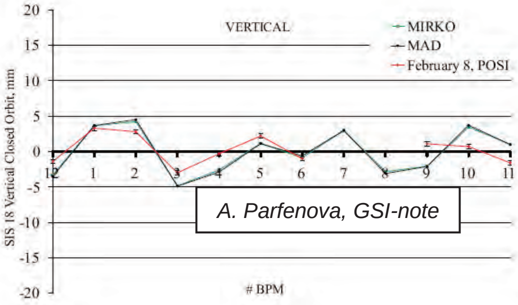
Validation of emittance growth and beam loss

experiment – simulation 10^5 turns ("frozen" space charge)



Origin of discrepancy:

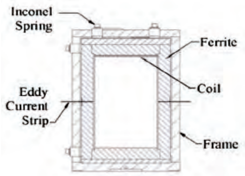
- factor ~2 underestimation of loss (similar to CERN-PS of 2002)
- poor representation of closed orbit → error strengths?
- sextupole strength only "indirectly determined" through low intensity loss?
- does lack of self-consistency matter?

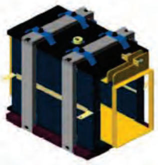


SNS –Ring (2006...2010):

Comparison of Experiment with ORBIT for coasting beam transverse instability (kicker)

1. Design phase of SNS: ORBIT compared with analytical model (code verification)
2. Comparison: measured impedance – experimentally determined from growth rates (code validation)





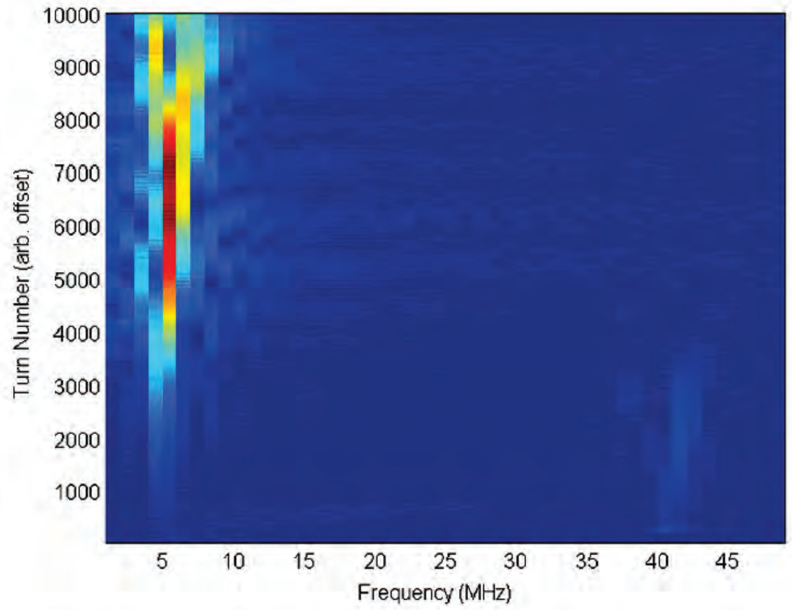


FIG. 7. Evolution of experimental turn-by-turn vertical harmonic spectrum of the extraction kicker instability.

simulated somewhat broader

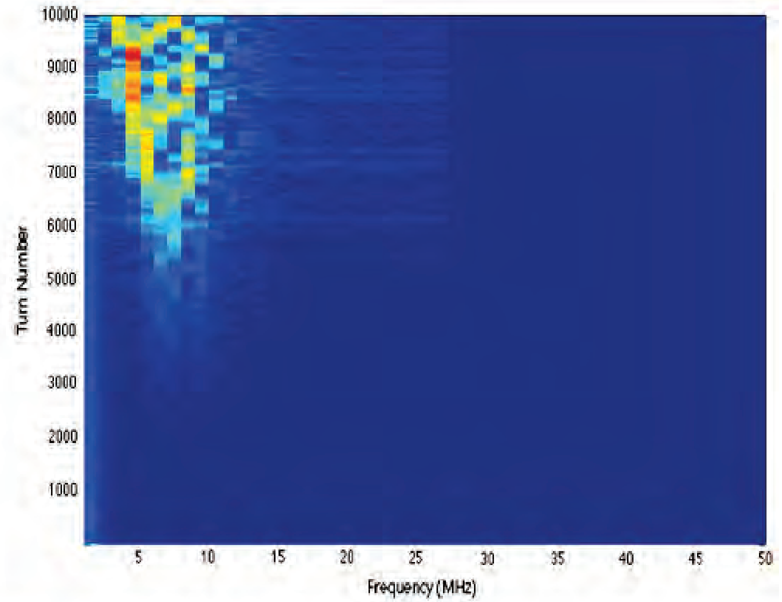


FIG. 9. Evolution of simulated turn-by-turn vertical harmonic spectrum of the extraction kicker instability.

Impedances

Estimates of kicker impedance
scaled from smallest kicker measurements (Hahn, 2004)

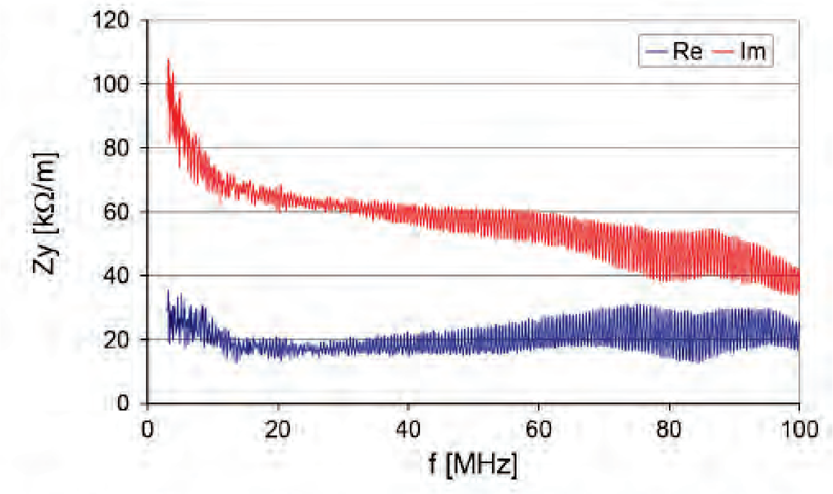


FIG. 2. Estimated coupling impedance of the SNS extraction kicker system, from Ref. [5].

Impedance simulations 2002/2003
used for ORBIT simulations

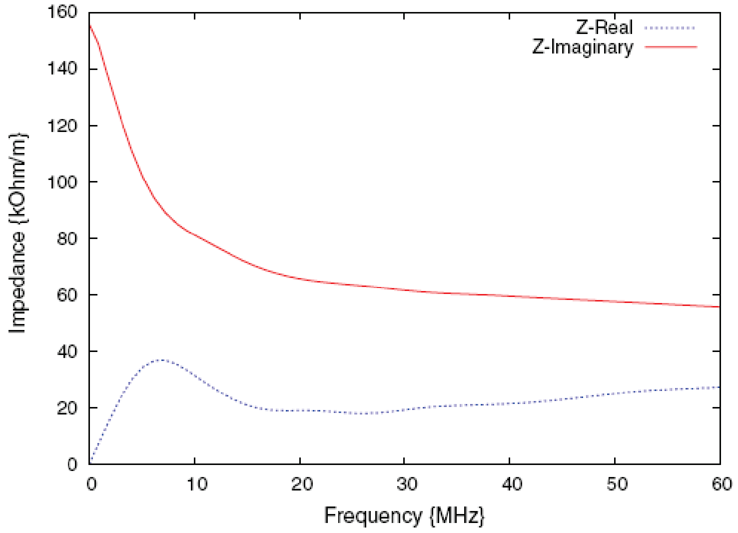


FIG. 3. Impedance of the SNS extraction kicker system used in simulations, based on Refs. [14,15].

SNS –Ring cont'd

1. Benchmarking of impedances at n=12:
   a. observed 1036 turns growth time for n=12
   b. derived 28 kΩ/m from observed growth time (assumed averaged β_{so} = 6m); agrees well with measured earlier 30 kΩ/m in laboratory
2. In ORBIT impedance from earlier measurement placed at β_{so} = 9.3 m
   a. simulation growth compares well with T=1036 from measurement

$$\mathrm{Re}\,(Z) = \frac{2\gamma\beta^2 E_0}{\tau\beta_{s_0} I}$$

No account of:
a. beam distribution
b. Landau damping
c. nonlinear regime

exponential growth time for n=12 in ORBIT consistent with measured growth time of 1036 turns (red line)

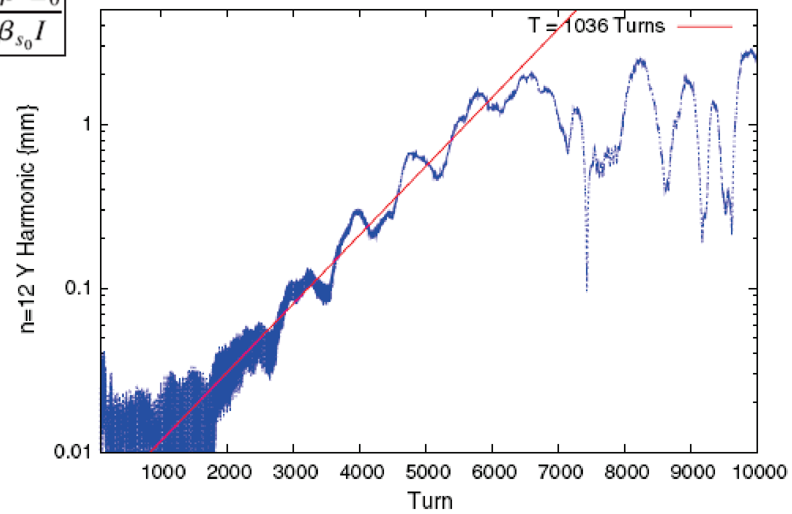


FIG. 8. Vertical $n = 12$ harmonic (in blue) versus turn number in the ORBIT extraction kicker instability simulation. The red line depicts an exponential growth time of 1036 turns.

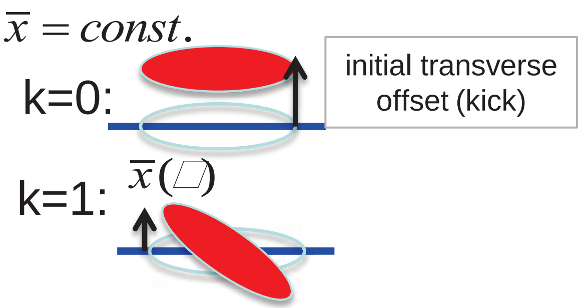
source: J.A. Holmes et al, PRSTAB 2011

Spectral information and high intensity

- could open a new window for direct benchmarking of space charge

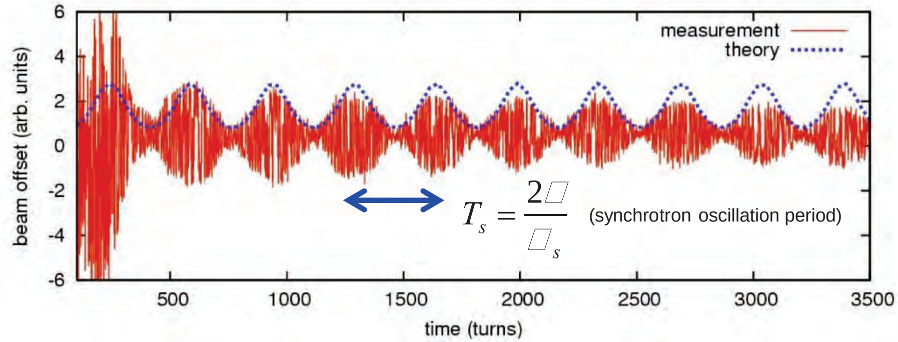
Recent work at SIS18 / PATRIC code

- initial transverse kick
- → need many synchrotron periods
- close interpretation by simulation



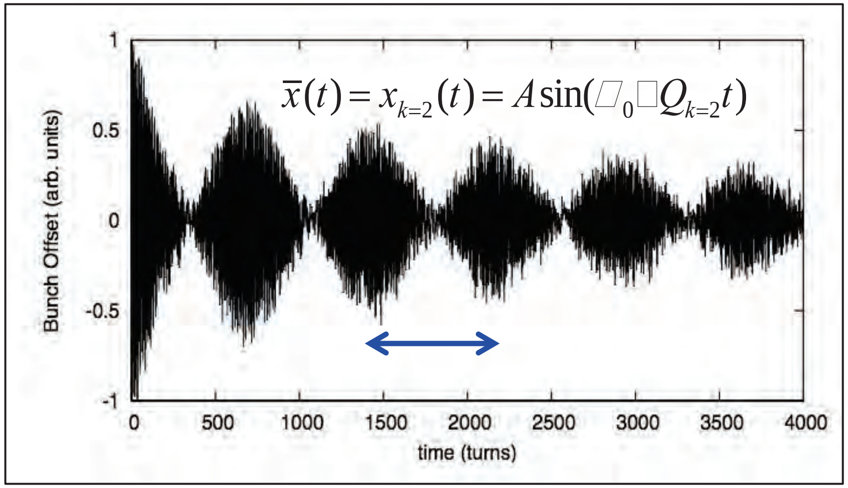
head-tail oscillations

Transverse de-coherence of head-tail oscillations (low intensity beams)



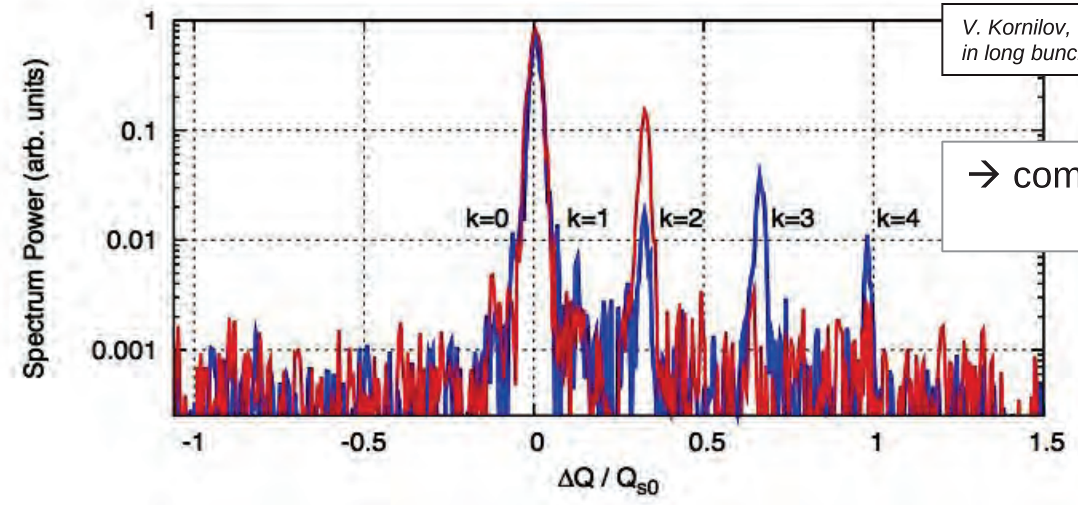
source: V. Kornilov

Measurement with ‘long’ Ar^{18+} bunches



FFT -> tune spectrum

Head-tail decoherence spectra + Landau damping

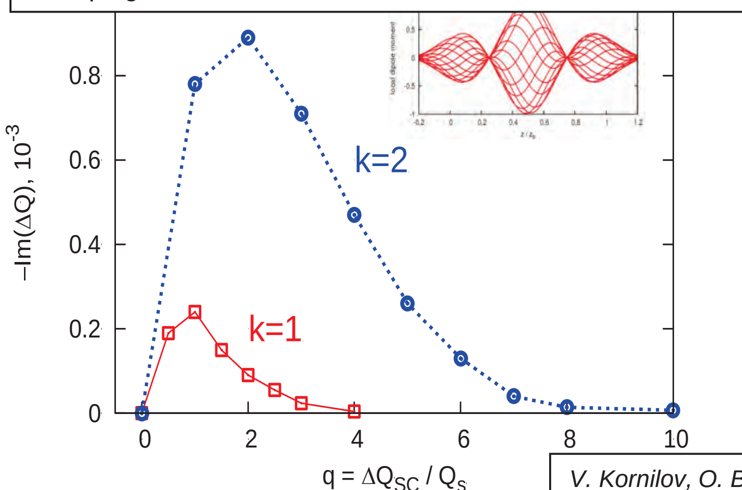


V. Kornilov, O. Boine-Frankenheim, Transverse decoherence and coherent spectra in long bunches with space charge, submitted to Phys. Rev. ST-AB

→ compare eigenfrequencies with simulation spectra
good collaboration diagnostics - theory!

Theory: A. Burov, Phys. Rev ST-AB (2009)
V. Balbekov, Phys. Rev. ST-AB (2009)

Damping rate of head-tail modes from **PATRIC simulation**



V. Kornilov, O. Boine-F., Phys. Rev. ST-AB (2010)

Landau damping reflects
- space charge
- bunch length

Further factors entering:
- distribution function
- impedances
- → **could become strongest test of simulation model vs. real model - needs work!**

Conclusions

- Point-wise progress has been achieved – "big" steps still to come
  - Verification of codes with idealized accelerator models in good shape → resolution of codes (grids, N) "good enough"
  - Good validation of some "intrinsic! physics mechanisms
  - Validation with real accelerators only slowly progressing
- Some common issues in linac and ring code benchmarking
  - Benchmarking not for single point in parameter space – need a significant knob!
  - Real lattice model is a problem – all kinds of errors needed
  - Closer interaction code developers – operation + diagnostics
- Differences linacs -rings
  - Linac space charge calculations "good enough"
  - in rings a problem for 10^5 ... 10^6 turns: "frozen-in" s.c. or self-consistent 2.5 D or 3D ?
  - initial distribution an issue in linacs (diagnostics problem)
  - distinction incoherent - coherent space charge not always clear (→ self-consistent?) - important for rings
- Future standards for benchmarking (linacs and rings)
  - accurate code model of real machine to support correction schemes
  - assist optimization of real machine

Direction quite clear, but still a long way to go!

GSI