LORASR CODE DEVELOPMENT

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Abstract

The LORASR code is specialized on the beam dynamics design of Separate Function DTL's based on the 'Combined 0 Degree Structure (KONUS)' beam dynamics concept. The code has been used for the beam dynamics design of several linacs which are in operation (GSI-HLI, GSI-HSI, CERN Linac 3, TRIUMF ISAC-I) or are scheduled to start beam operation in the near future (Heidelberg Therapy Injector, HITRAP Decelerator, GSI Proton Linac). The recent code development was focused on the implementation of a new PIC 3D FFT space charge routine, allowing for time-efficient simulations with up to 10^6 macro particles routinely, as well as of tools for error studies and loss profile investigations. The LORASR code was successfully validated within the European 'HIPPI' Project activities. The error study tools are a stringent necessity for the design of future high intensity linacs. The new LORASR release will allow particle loss studies during the design of the GSI FAIR Facility Proton Linac, as well as detailed transmission investigations on the IFMIF Accelerator. This paper presents the status of the LORASR code development and the benchmarking results.

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LORASR CODE FEATURES AND APPLICATIONS

The LORASR code can treat all kind of drift tube structures, but is especially well suited for the design of KONUS lattices [1]. A KONUS period consists of a quadrupole triplet lens, a rebuncher section at negative synchronous phase and a multi cell zero degree synchronous particle main acceleration section. This concept is especially effective if applied for accelerator designs using βλ/2-type H-mode resonators with 'slim' drift tubes which carry no focusing elements.

The LORASR code provides the single particle tracking along drift tube sections, quadrupole lenses, short RFQ sections including fringe fields and dipole magnets. The electric gap field components are defined by a parametric input data set, valid for 10 gap geometries with different gap length to inner diameter ratios. Datasets are available for 'slim' tube geometries (aperture ratio r_o/r_i = 1.4 typically) as well as for "Alvarez-type" thick tubes. The latest have been calculated by Microwave Studio™.

Recent code development was concentrated on the following items:

- Implementation of a new space charge routine based on a PIC 3D FFT algorithm.
- Implementation of a 'particle breeding' routine used for increasing the number of simulation particles available from original RFQ output distributions.
- Implementation of tools for error study and loss profile investigations.

Moreover, the LORASR code was included in the Poisson solver benchmarking and tracking comparison programme within the 'High Intensity Pulsed Proton Injector' (HIPPI) European network activity [2].

Characteristic applications making use of the upgraded LORASR code features are high current, low and medium energy linac designs with stringent particle loss requirements. Two significant examples are the beam dynamics design of the 70 mA, 3-70 MeV Proton Injector for the GSI FAIR Facility [3], [4] and the IAP proposal of a 125 mA D^+, 5-40 MeV superconducting CH-DTL section for the International Fusion Materials Irradiation Facility (IFMIF) [5].

NEW LORASR ROUTINES AND ENHANCED CODE CAPABILITIES

New PIC 3D FFT Space Charge Solver

The main steps of the new LORASR Particle-In-Cell (PIC) space charge solver are:

- Charge density deposition of an arbitrary macro particle distribution to a Cartesian 3D grid.
- Fourier expansion of the grid charge density $\rho_{i,j,k}$ by using a FFT algorithm.
- Calculation of the potential values $U_{i,j,k}$ by solving the Poisson equation on the grid.
- Calculation of the electric field values from the grid-defined potential and interpolation of the field values to the exact particle positions.

The advantage of this method is that the FFT algorithm recursively breaks down a discrete Fourier transform (DFT) of composite size $N = n_1 \times n_2$ into smaller DFTs of sizes n_1 and n_2 and thus reduces the number of arithmetical operations from the order N^2 to the order $N \bullet \log_2 N$.

Presently an algorithm using closed boundary conditions (Dirichlet cond. for the potential at the surface of a rectangular pipe, up to 128 x 128 x 128 grid points, up to 1 million macro particles) is implemented.

Routine for Enhancing ("Breeding)" the Macro Particles Number from RFQ Simulations

Output distributions available from RFQ simulations usually have less macro particles than could be processed by LORASR, taking advantage of the new FFT based space charge routine. A major concern from the point of view of the DTL design is to quantify the percentage of particle losses along the accelerator by using as many simulation particles as possible. This is why a

combination of many macro particles together with realistic RFQ output distributions is the most attractive solution, if available.

An accurate solution would be to sum up the particle distributions generated from several RFQ runs. For the purpose mentioned before, a faster solution is to artificially enhance the number of macro particles available from RFQ simulations. This could be done by calculating the density of the initial particle distribution in the 6D phase space $f[x_1,..,x_6]_N$ and filling every cell of the 6D space correspondingly. This method fails when the initial particle number N is too low (like 3808 particles in the given example). Any other method used has to meet the following constraints:

- The coupling between 2-dim subspaces must be conserved - they cannot be populated independently.
- Fixed beam parameters have to be defined, e.g. the rms emittance of the initial and final distributions.

Considering these constraints, the following particle 'cloning' procedure was developed:

- New particles are generated with coordinates identical to the 'parents' in all 6 dimensions.
- 'Child' particles are randomly (Gaussian) shifted in each 2-dim subspace, within radii corresponding to the local particle density. In a final step an additional particle 'scattering' procedure is applied, in order to avoid artificial local clustering.
- Fitting of the resulting rms emittances by an iterative process, until they are close enough to the values of the initial distributions ($\Delta\varepsilon < 1‰$).

An example of the results achieved by the 'breeding' algorithm is shown in figure 1:

Code Efficiency Benchmarking and Validation of the Particle Breeding Routine

In order to both validate the particle breeding routine and check the performance of the new LORASR PIC 3D FFT routine, the present design lattice of the GSI 3-70 MeV, 70 mA Proton Linac DTL was used for LORASR calculations with original RFQ output distribution data (3808 macro particles) and artificially added particles (up to 10^5 total particle number).

The results are illustrated by figure 2 and table 1.

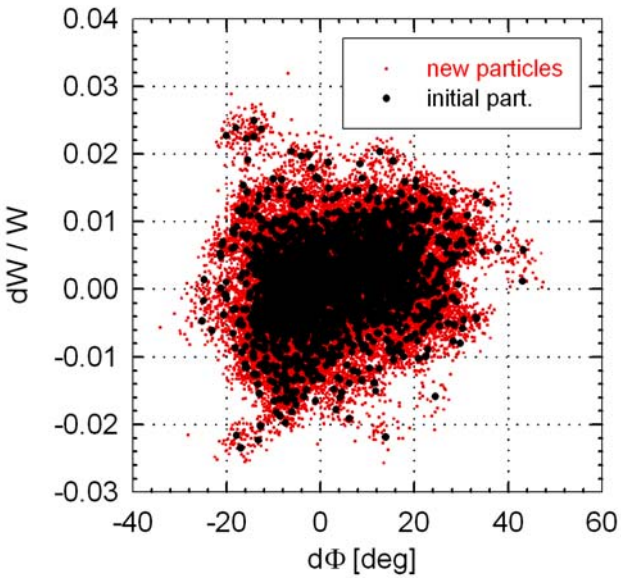

Figure 1: Example for 'particle breeding' routine results. 100000 particles were generated out of 3808.

- **Code performance**:

The theoretically expected FFT algorithm processing time is ~ ($N_{particles} + N_{meshpoints} \times \log_2 N_{meshpoints}$).

The actual running times (column 3 of table 1) however show an almost linear dependency: $t_{s.c.routine} \sim N_{particles}$. This is because in practice the elementary operations (loops) depending on the particle number are predominant towards the (~ $N_{meshpoints}$ dependent) FFT algorithm itself.

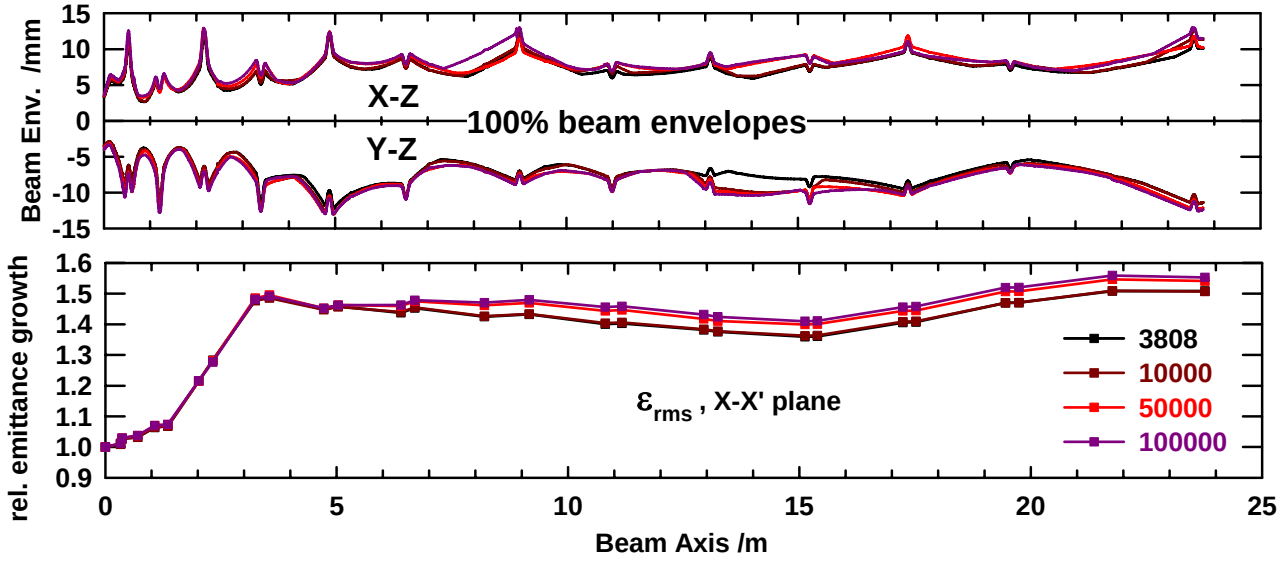

Figure 2: DTL design lattice used for LORASR code performance tests and for the validation of the particle breeding routine: GSI 3-70 MeV, 70 mA Proton Linac DTL calculated with original RFQ output distribution data (3808 particles) and different numbers of artificially added particles.

Table 1: LORASR Code Performance Test
(No. of space charge calls: 982)

Part. No., input	Part. No., exit	CPU Time / s.c. call [s]	Total CPU Time [s] (% used by s.c. routine)
3808	3808	0.043	62.2 s (67.9 %)
10000	10000	0.091	133 s (67.3 %)
50000	49993	0.562	746 s (74.0 %)
100000	99975	0.955	1293 s (72.5 %)

The step in the linearity of CPU times observed at the transition from 10^4 to 5×10^4 particles is due to the adaptive fitting of the mesh point number: 32^3 for $N_p \leq 10^4$, 64^3 for $N_p \leq 10^5$ and 128^3 for $N_p \leq 10^6$, respectively. The new s.c. routine still needs the major part of the total calculation time. However, due to the nearly linear dependency on the particle number, validation runs with 10^6 macro particles are now routinely available, resulting into total CPU times below 4 hours on a modern PC with a 3 GHz CPU for the given GSI Proton Linac example.

- **Validation of the particle breeding routine**:

As seen from figure 2, the particles artificially added to the initial RFQ output distribution only marginally influence the beam dynamics results. The differences in the 100% transverse beam envelopes and rms emittances are only due to single particle effects. Nevertheless, the behaviour of the emittance growth along the lattice is comparable for the different runs, even when the initial (3808) and final (10^5) particle numbers differ a lot.

As expected, particle losses are observed for larger simulation particle numbers only ($>5\times10^4$). This improved 'resolution' in simulation is a stringent necessity for future detailed particle loss profile investigations.

BENCHMARKING RESULTS WITH LORASR WITHIN 'HIPPI'

Within the framework of the HIPPI project [2], LORASR was successfully included to the Poisson solver benchmarking and tracking comparison programme. An overview on the aims and present results of this European Framework Activity is available from the Web site [6] and the corresponding publications [7],[8].

Therefore in this paper only a representative example on the attained degree of accordance between the results of the participating codes is given (see figure 3).

Especially the validation of the new LORASR space charge routine within the HIPPI Static Poisson Solver and Single Particle Tune Comparison Programme was very successful and a good opportunity for testing the in-house code developments within a broader developer community.

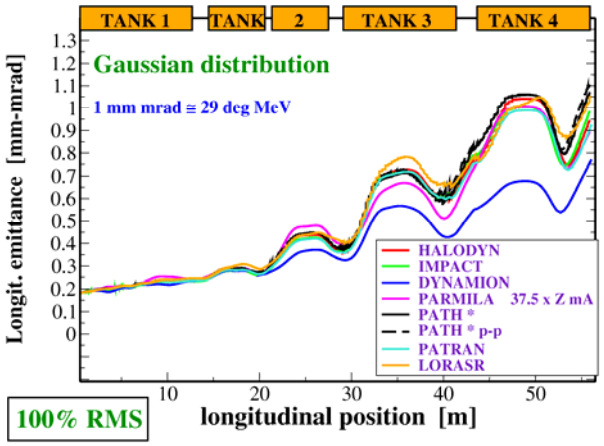

Figure 3: Example of UNILAC Alvarez section tracking code comparison results within the 'HIPPI' collaboration (courtesy of A.Franchi [6]). Parameters: $^{238}U^{28+}$, I_{beam} = 37.5 mA, W_{in}=1.4 AMeV, 6D Gaussian bunch, not matched.

ACKNOWLEDGEMENT

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