CSRtrack: FASTER CALCULATION OF 3-D CSR EFFECTS

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Abstract

CSRtrack is a new code for the simulation of Coherent Synchrotron Radiation effects on the beam dynamics of linear accelerators. It incorporates the physics of our previous code, TraFiC4 [1], and adds new algorithms for the calculation of the CSR fields. A one-dimensional projected method allows quick estimates and a greens function method allows 3-D calculations about hundred times faster than with the 'direct' method for large particle numbers.

The tracking code is written in standard FORTRAN77 and has its own parser for comfortable input of calculation parameters and geometry. Phase space input and the analysis of the traced particle distribution is done with MATLAB interface programs.

INTRODUCTION

In usual optics and tracking codes for accelerator development the bunch self fields due to synchrotron radiation and changes of the bunch shape are neglected. Therefore special CSR tracking codes have been developed (e.g., TraFiC4 [1], CSRtrack, R.Li's code [2]) and existing codes have been expanded (e.g., Elegant [3,5], TREDI [4]). Essentially two types of approaches are presently used for the self-consistent calculation of particle distributions on curved trajectories. Both are available in CSRtrack.

The 1-D approach uses a simplified model for the calculation of longitudinal forces [6]. It neglects transverse forces as well as transverse beam dimensions and assumes that the longitudinal distribution is unchanged at retarded times. A 'renormalized' Coulomb term is used to extract the field singularity in the 1-D beam.

The sub-bunch approach uses a set of 3-D charge distributions*, e.g., time-independent Gaussian, to approximate the source distribution. The physical model of the sub-bunch method is complete, but the resolution of phase space modelling is severely limited by the numerical effort for the field calculation of all point to point interactions. Even with parallel computing particle numbers above 10^3 are difficult to handle (CPU time on a cluster is many days).

TraFiC4 and CSRtrack ease that problem by using a convolution method [8] to reduce the field calculation of 3-D sources to 1-D integrations (for each interaction), gaining about a factor of ten in manageable particle numbers.

Further improvement is possible with a pseudo Green's function approach; it uses the discretized field of one reference sub-bunch to calculate all interactions. This method is implemented in CSRtrack and allows tracking calculations with 10^4 particles on one CPU in a few hours, up to $4 \cdot 10^4$ particles have been tracked on 20 CPUs.

For the tracking of even bigger numbers of particles, the disadvantage that the effort scales quadratic with the number of particles could be avoided by calculating the electromagnetic fields on a mesh. With a combination of mesh field calculation and pseudo Green's function method, $>10^5$ particles in less then one day (using 20 CPUs in parallel) seem to be in reach.

NUMERICAL ASPECTS OF DIFFERENT CSR FIELD CALCULATION METHODS

In the following we discuss different algorithms and their relative computation time consumption, which are summarized in Fig. 2.

A word of warning: if the initial bunch density is modulated, for instance to study CSR induced instability, the computation time depends quadratically on the ratio of the bunch length to its fine structure – in any approach. We will discuss that further in a paper to come.

One Dimensional Approach – Projected Method

The particle distribution is projected to the reference trajectory and a smooth one dimensional charge density $\lambda(s)$ is calculated by binning or filtering. The smoothing is crucial for the stability and accuracy of the simulation because the micro bunch instability is sensitive to high frequency components in the charge density.

The longitudinal field $E^{(\lambda)}$ can be calculated by one dimensional integration

$$E^{(\lambda)}(s_0,t_0) = \int \lambda'(u + s_0 - vt_0) K(s_0,u) du\,,$$

with the kernel function $K(s_0,u)$ that depends on the geometry of the trajectory. This integral is a convolution in time. It can be solved efficiently by FFT methods if $E^{(\lambda)}$ is required for a time interval.

The longitudinal field is calculated on a mesh and interpolated to the projected particle positions. The particle tracking takes into account external fields and the longitudinal self field. The effort for the field calculation depends linearly on the number of particles.

Sub-Bunch Approach

The distribution of source particles is described by a set of sub-bunches with well defined shape. The individual trajectory of each sub-bunch has to be known in absolute coordinates back in time. This defines the 3-D source distribution $\rho(\mathbf{r},t)$ so that potentials and electromagnetic fields can be calculated by an integration of retarded sources.

A disadvantage of the sub-bunch approach is the large numerical effort. For M test particles and N source distributions (sub-bunches) $M \times N$ three-dimensional integrations have to be performed for every time step.

* 2-D sub-bunches in R.Li's code

Source Distributions and Test Particles

For **self consistent tracking** the trajectory of each source is defined by the motion of an associated test particle. Therefore $M=N+M_t$ test particles are needed, with M_t the number of additional particles that can be used for more detailed explorations e.g. of the transverse phase space. The effort for self consistent tracking is at least proportional to N^2. Additional test particles need the computation of $N\times M_t$ interactions.

If the bunch shape is weakly deformed due to self forces a **perturbation approach** can be used. The self forces to the test particles are calculated for unperturbed motion of source distributions and test particles. These forces are used in a second step to calculate the perturbed motion. The initial condition of test particles can be set as required (e.g. to investigate an individual slice) but at least some test particles should be used to verify the perturbation approach.

3-D Sub-Bunches, Convolution Method

Since the field of each source sub-bunch has to be calculated for every test position by a 3-D integration of retarded sources, the full field computations is quite time consuming. For spherical Gaussian sub-bunches this integration can be reduced to a 1-D integral [7].

The codes TraFiC4 and CSRtrack adopt a calculation method that was developed in [8]. A certain type of 3-D distribution can be represented by the convolution of a longitudinal 1-D profile $\lambda(s,t)$ with a transverse 2-D density function $\eta(x,y)$.

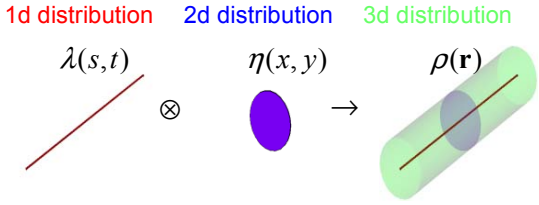

Fig 1: *Schematic of the Convolution Method*

Then the 3-D electromagnetic fields can also calculated by a convolution of fields $\mathbf{E}^{(\lambda)}$, $\mathbf{B}^{(\lambda)}$ caused by the 1-D source with the 2-D density function. $\mathbf{E}^{(\lambda)}$ and $\mathbf{B}^{(\lambda)}$ are split into singular parts $\mathbf{E}^{(\lambda,s)}$ and $\mathbf{B}^{(\lambda,s)}$, which are dominated by local effects, and non-singular parts $\mathbf{E}^{(\lambda,ns)}$ and $\mathbf{B}^{(\lambda,ns)}$. The asymptotic behaviour of the singular part is analytically known so that its convolution with certain transverse density functions can be computed efficiently.

As the non singular parts depend mainly on long range interactions, their transverse dependency is weak and the convolutions $\mathbf{E}^{(\lambda,ns)}\otimes\eta$, $\mathbf{B}^{(\lambda,ns)}\otimes\eta$ can be approximated by $\mathbf{E}^{(\lambda,ns)}$, $\mathbf{B}^{(\lambda,ns)}$ for sufficiently small transverse dimensions ($<<\sqrt[3]{R_0\sigma_\lambda^2}$, with R_0 the curvature radius and σ_λ the bunch length). Therefore the numerical effort E_c is determined by the 1-D integration for the non singular parts. The total effort for all source to test-point interactions is $M\times N\times E_c$.

Pseudo Green's Function Approach

The fields $\mathbf{E}^{(0)}(\mathbf{r},t_0)$, $\mathbf{B}^{(0)}(\mathbf{r},t_0)$ of a reference sub-bunch (charge q_0) that travels along a reference trajectory $\mathbf{r}_0(t)$ are used to approximate the fields of other sub-bunches (charge q_ν, trajectory $\mathbf{r}_\nu(t)$). This approach neglects vertical forces. At the observation time t_0 the trajectory of sub-bunch ν is approximated by

$$\mathbf{r}_\nu(t) \approx \mathbf{r}_\nu(t_0) + \mathbf{R}\cdot\left(\mathbf{r}_0(t)-\mathbf{r}_0(t_0)\right).$$

This shift-rotation-transformation (with rotation operator $\mathbf{R}$) is used to calculate

$$\mathbf{E}^{(\nu)}(\mathbf{r},t_0) \approx \frac{q_\nu}{q_0}\mathbf{R}\cdot\mathbf{E}^{(0)}\left(\mathbf{r}_0(t_0)+\mathbf{R}^{-1}(\mathbf{r}-\mathbf{r}_\nu(t_0)),t_0\right)$$

and $\mathbf{B}^{(\nu)}(\mathbf{r},t_0)$ in the same way. The pseudo Green's functions $\mathbf{E}^{(0)}(\mathbf{r},t_0)$, $\mathbf{B}^{(0)}(\mathbf{r},t_0)$ are calculated once for every time step on a 2-D mesh in the horizontal plane with M_g points:

$$\mathbf{E}^{(0)}(\mathbf{r},t_0) = E_x(x,y)\mathbf{u}_x + E_y(x,y)\mathbf{u}_y$$

$$\mathbf{B}^{(0)}(\mathbf{r},t_0) = B_z(x,y)\mathbf{u}_z$$

The numerical effort for the calculation of all self forces is $M_g\times E_c+M\times N\times E_{i,g}$ with $E_{i,g}$ the effort for the interpolation on the mesh. The approach is effective for $N\times M > M_g$. Simulations with many particles ($>10^4$) are not limited by the effort for the field calculation ($M_g\times E_c$) but by the effort for the interpolation ($M\times N\times E_{i,g}$).

Meshed EM Fields

If the density of particles is large compared to the fine structure of the particle distribution (and the self-fields) it is more efficient to calculate electromagnetic fields on a mesh with M_{em} points and to interpolate them to the test points. The numerical effort is $M_{em}\times N\times E_c+M\times E_{i,em}$ with $E_{i,em}$ the effort for the interpolation on the field mesh. The total effort is not longer proportional to the squared number of particles ($M\times N$ with $M \geq N$ for self consistent tracking)!

Reasonable EM meshes need at least $M_{em} > 10^4$ points and therefore the method gets efficient for M, $N > 10^4$. The effort for such particle numbers is still too large (even with parallel computing) for routine investigations.

This is different if the meshed fields approach is combined with the pseudo Green's function approach: the total effort is $M_g\times E_c+M_{em}\times N\times E_{i,g}+ M\times E_{i,em}$. This method is still in preparation.

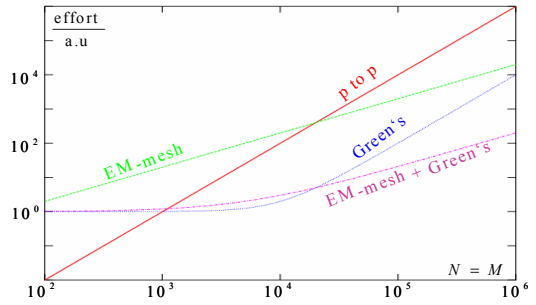

Fig. 2: *Numerical effort of different CSR field calculation methods vs. # of tracked particles*

Iterative Tracking

For tracking, self-forces have to be calculated for particles on phase space coordinates that depend on the unknown forces. If the track step is sufficiently small the forces can be approximated for phase space positions calculated without self contributions. To avoid the numerical effort for very many small steps iterative tracking with medium step size is used: estimated self forces are calculated for estimated particle positions and are used to improve the position estimation. The iteration is repeated until an error criterion is fulfilled.

The numerical integration of the equation of motion in CSRtrack uses sub-steps that are (much) smaller than the steps of the iterative force calculation. The forces at sub-steps are linearly interpolated between the force at the start point of an iterative step and at its end point. The error due to this linear interpolation and due to too big iterative steps is not reduced by iterative tracking.

CSRtrack provides two possibilities to determine the size of iterative steps: by a recursive algorithm that is based on the bunch length and curvature radius of the trajectory and by external definition. Like in all self-field applying tracking codes, the result has to some extent to be interpreted and justified by the user (e.g. convergence tests or the inspection of the forces observed by some selected test particles).

CSRtrack 1.0

Particles Definition

Position, momentum and charge of each particle of the distribution are defined in an absolute Cartesian coordinate system with the horizontal plane as *xy*-plane. Particles with nonzero charge are source particles that create self-fields that affect the motion of test particles. In the present versions all particles have the source and test property.

Lattice

CSRtrack supports magnetic dipole- and multipole-fields that are defined in Cartesian coordinates. The range of the fields of one element is limited by two field boundaries perpendicular to the horizontal plane. The **dipole** field between two field boundaries is constant and parallel to the vertical *z*-axis. Together with the dipoles a reference trajectory is defined that consists of arcs and lines.

To take into account vertical edge focussing at the hard edges of dipoles the tracking algorithm applies discrete kicks proportional to the vertical offset. The magnetic **multipole** field is defined in a local coordinate system (longitudinal, horizontal, vertical) with its origin in the intersection point of the reference trajectory and the field boundary.

The magnetic multipole field between field boundaries depends only on transverse coordinates. It is characterized by its strength, azimuthal order, transverse offset and skew angle.

Shielding

CSRtrack provides shielding as of now with parallel ideal conducting plates with constant distance to the beam. The user has to specify the maximum distance to the beam up to which mirror charges will be taken into account.

Parallel Computing

CSRtrack is available as a parallel processing code using the MPI protocol with the MPICH package. Only the sub-bunch methods are calculating parallel.

# of particles	calc. steps	Method	CPU	Running time
10000	~200	Point to point	20x1GHz	~ 10 d
10000	~200	Greens funct.	1x1GHz	~0.5 d
41000	~200	Greens funct.	20x1GHz	~0.5 d

Table 1: *CPU time consumption of CSRtrack runs for TTF2 and XFEL magnet chicanes*

COMPARING RESULTS FOR DIFFERENT METHODS

CSRtrack is well suited to explore the applicability of different CSR calculation methods. An example is a calculation for the European XFEL bunch compression system (see Fig. 4).

The beam is tracked from the gun into the linac up to about the 100 MeV point with a space charge code (ASTRA). For the remaining injector linac up to the two magnetic chicanes for bunch compression a linac tracking code (elegant) is used. In the chicanes, where the beam dynamics is dominated by CSR effects, we need to employ CSRtrack.

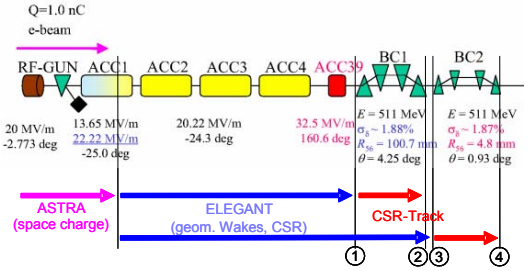

Fig. 4: *Start-to-end calculation for the European XFEL*

In Fig. 5 the longitudinal phase space at the end of the beam line is shown; calculated with the 1-D and a 3-D method of CSRtrack. The RMS bunch length is about 20 μm, the peak current 5 kA.

The longitudinal tails of the initial distribution have been over-compressed back towards the center of the distribution. They have to be excluded from any meaningful evaluation of beam parameters vs. longitudinal bunch position such as transverse slice emittance or, as shown here, slice energy spread. In the graphs, these particles are color coded.

The 1-D model underestimates the growth in slice energy spread in the center of the bunch due to CSR effects by a factor of 5-10.

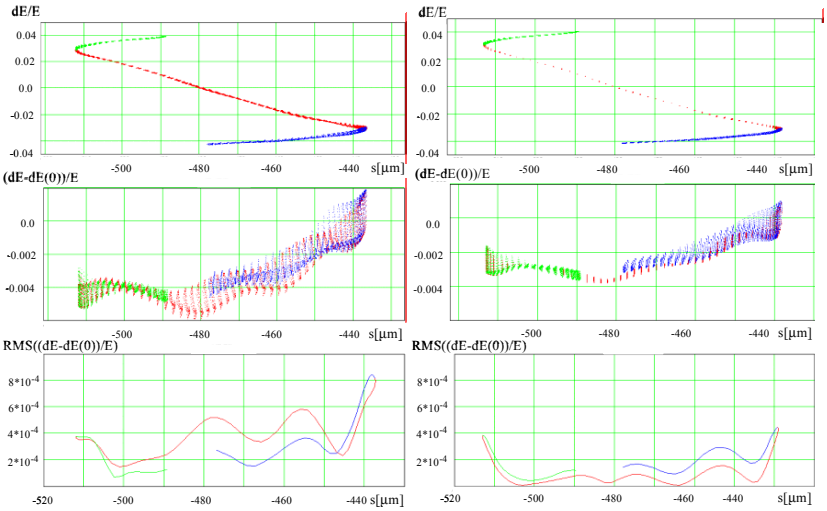

Fig. 5: *Longitudinal Phase Space at the end of the bunch compression system calculated with the 3-D Greens function method (left) and the projected 1-D method (right).*

The lower graphs show the difference in particle energies due to compression and the RMS of that value vs. longitudinal bunch position.

The particles in the energy distribution tails are shown in blue and green.

POSTPROCESSING

We use MATLAB tools on a XP PC to administrate and manipulate the data files and to run the tracking codes on both the local (XP) computer and a Linux PC cluster, in single CPU or parallel processing mode (see Fig. 6).

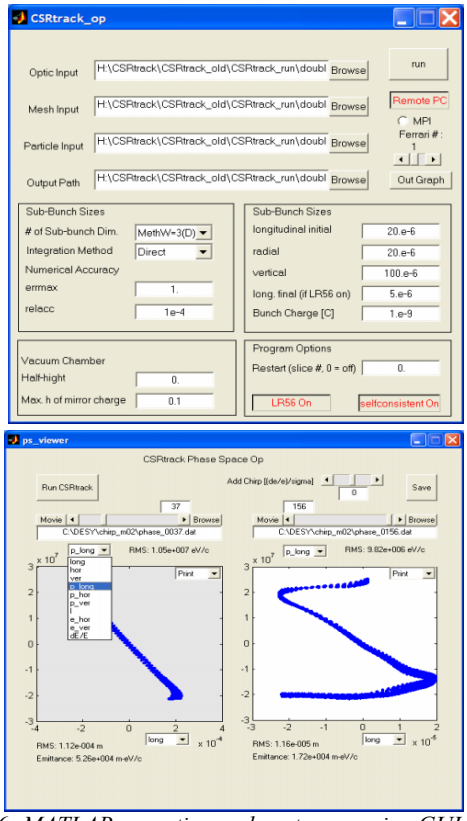

Fig.6: *MATLAB operating and post-processing GUIs*

Input and output phase space data files can be inspected, changed and plotted.

User options are made invisible if they do not make sense; for example the option to display beam current (I) on the vertical axis disappears if something else than the longitudinal coordinate is chosen for the horizontal axis.

File formats are checked and detected automatically to avoid mistakes. Saving data in files works via the standard XP 'save as' window, also the file formats (e.g., elegant or ASTRA) can be chosen with the familiar pull-down menu.

FURTHER PLANS, CONCLUSION

Soon a web page will be ready to download a CSRtrack executable and a user's guide with input examples. The program has to be developed further to incorporate the mesh option described above.

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