Remarks on the Road Map:

- **Computing CSR and space charge fields: advantages of the frequency domain with account of vacuum chamber**
- **Smoothing of particle distributions to make sources for the wave equation**
- **Nonlinear Vlasov solutions vs. macro-particle simulation**

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I. REQUIREMENTS OF A GOOD CODE FOR CSR AND SPACE CHARGE

Coherent synchrotron radiation (CSR) and appreciable space charge forces are features, often detrimental, in most advanced accelerator projects. For designing of new machines and to understand the phenomena in existing machines it would be highly desirable to have a code with at least the following properties:

1. Source particles close to a planar reference orbit consisting of an arbitrary sequence of bends and straights. Option to include undulator orbits as well.

2. A quasi-realistic vacuum chamber following the reference orbit, for instance a rectangular perfectly conducting chamber of constant height (but possibly varying width). Straight vacuum chamber in the case of an undulator.

3. An arbitrary phase space distribution in the CSR source (6D, 4D) and corresponding charge/current distribution (3D, 2D).

4. The possibility of self-consistency, allowing for evolution of the bunch under its self-force, conditioned by electromagnetic boundary conditions on the chamber walls.

5. The ability to handle very short bunches, maybe even to sub-micron size.

6. Full field calculation including longitudinal and transverse wake fields and space charge, allowing non-relativistic particles. Option to compute the fields at any point in the vacuum chamber, thus allowing study of the resistive wall effects and modeling of off-axis field observations.

7. Reasonably fast turn-around on modest hardware (few CPU's, low-end GPU).

8. Convenient to use without extensive study.

9. Reliable and robust regarding numerical convergence issues.

10. Integration with a general accelerator code environment such as Bmad.

At present no code comes close to fulfilling all these requirements. The most useful appears to be **elegant**, which gives a very good first cut but allows only a one-dimensional description of the charge/current source of CSR, as determined by projection from a 6D

distribution of macro-particles. Limitations of this model have been observed, and are likely to be increasingly evident in more demanding problems.

II. FREQUENCY DOMAIN FORMULATION WITH VACUUM CHAMBER

I believe that there is a strikingly simple path toward a code having all of the properties listed. It goes back to work of Stupakov and Kotelnikov [1] and Agoh and Yokoya [2], but with essential modifications. It is also closely related to my work with Morton [3] on CSR in a rectangular toroidal chamber, and is in fact a natural generalization of that work.

The scheme works exclusively in a rectangular chamber of fixed height h. (Working in the parallel plate model or in free space would be much more difficult from my viewpoint, besides losing some essential physics.) The first step is to replace the variable pair (s,t) by (s,z), where $z = s - \beta ct$ is the beam frame coordinate. The next step is to take the Fourier transform of the Maxwell equations and sources with respect to z, and to invoke a Fourier series in the vertical coordinate y, in such a way as to meet the boundary conditions on the top and bottom of the chamber. After the transforms all field components and sources depend on the four variables (k, α_p, x, s), where k is the continuous wave number conjugate to z, and $\alpha_p,\ p = 1, 2, \cdots$ is the discrete wave number conjugate y. **It is very important not to make a Fourier development in x, as was done in Ref. [1].**

Now a great simplification arises from the fact that all six components of the electromagnetic field can be expressed algebraically in terms of just $\hat{E}_y$ and $\hat{H}_y$ and their derivatives with respect to x and s. The 2D wave equations for those two fields have a very simple form, if we use polar coordinates in bends and Cartesian coordinates in straights. The derivatives involved are $\partial/\partial s,\ \partial^2/\partial s^2,\ \partial/\partial x,\ \partial^2/\partial x^2$. The x-derivatives will be represented in terms of divided differences on a mesh, say with the simplest choice of a 3-point rule, which turns out to be quite adequate. **Values on the x-mesh are set up in such a way that the EM boundary conditions on the vertical walls of the chamber are met automatically.**

III. REDUCTION TO A SYSTEM OF LINEAR ORDINARY DIFFERENTIAL EQUATIONS

In the first instance we throw away the terms in $\partial^2/\partial s^2$. This corresponds to the paraxial approximation used in Refs.[1, 2]. Then for given sources the computation consists of integrating a system of linear ordinary differential equations (ODE's) of the form

$$\frac{dF}{ds} = A(s)F + S \ , \tag{1}$$

where F is a complex vector consisting of the values of the field at the x mesh points x_i, and the source term S is also a complex vector. In fact there are two independent systems (1), one for the electric field with $F_i = \hat{E}_y(k, \alpha_p, x_i, s)$ and one for the magnetic field with $F_i = \hat{H}_y(k, \alpha_p, x_i, s)$. The matrix $A(s)$ comes from discretizing the wave operator on the x-mesh, and in a bend that is just the familiar operator of the Bessel equation, which is computed very quickly in its discretized form.

In the simplified model studied to date the charge/current source is a vertical ribbon beam [3], so that the source for E_y contains a $\delta(x)$ and the source for H_y contains $\delta'(x)$. **To handle this situation numerically, I take the important step of changing the independent variable F to a new variable $\tilde{F}$, in such a way that the new effective source $\tilde{S}$ is a smooth function of x, spread over the entire width of the chamber [4].** Correspondingly, $\tilde{F}$ is also smoother than F, and a good object for numerical approximation. This change of variable generalizes to a realistic source, such as would be involved in a macro-particle simulation, thus spreading out and smoothing a source first concentrated at small x.

IV. FAST INTEGRATION OF THE DIFFERENTIAL EQUATIONS

After the change of variable the system (1) is to be integrated as an initial value problem, step-wise in s through any succession of bends and straights, for each choice of the wave numbers (k, α_p). An immediate question is the required range of k and α_p; is it small enough to be manageable? A positive answer came out in a first implementation of the method in Ref.[4]. For k there is the so-called shielding cutoff at small k, which appears in the same way as it did in the full torus [3], owing to the properties of the Bessel operator. The cutoff at large k is at least the reciprocal of the r.m.s. bunch length and usually needs to

be appreciably larger than that to account for non-Gaussian substructure. An acceptable increment Δk on the mesh in k is not immediately known, but is soon determined empirically. As for the vertical mode number, it has been known since Ref.[3] that only a few modes should be required; in fact this motivated the very useful Fourier expansion in y.

The work of [4] and [5] showed that the necessary range of (k, α_p) can be handled quite comfortably. Since the inverse Fourier transforms to get back to space-time are not costly, I claim that the frequency domain formulation in this guise is eminently practical.

In [4] we used an explicit integrator (leap frog rule) for solving (1). This required very small steps in s for stability, but nevertheless was impressively fast. In [5] I showed that an implicit integrator, the trapezoidal Crank-Nicolson method, could give a large net speed-up. Although the time per step is somewhat larger, the steps in s can be very much bigger, for instance by a factor of 350. In a recent trial for the parameters of LCLS-II, BC2, which has a 10 micron bunch length, I integrate through one bend of the bunch compressor for all required values of (k, α_p). **The CPU time is 1.7 sec. (Here and in the following, times are for a serial code in Fortran running on a laptop). Moreover, the code is very simple, comprised of 300 lines, mostly for set-up of preliminaries.** The run included 100 values of k with $k_{\max}\sigma_z = 10$. There were 5 values of α_p, while the mesh in x had 301 points. There were 300 steps in s, and the longitudinal wake field was computed at every s-step. The wake field showed convergence with this choice of discretization parameters.

V. PLAN FOR A REALISTIC AND SELF-CONSISTENT SIMULATION

Aside from the splendid results on timing, a further very important advantage of the scheme is its weak dependence on the dimension and complexity of the source, as far as solution of the field equations is concerned. Given the effective charge/current source $\tilde{S}(k, \alpha_p, x, s)$ the solution of the field equations will take a time not too different from that just mentioned, whether the source has a 1D, 2D, or 3D description in space-time. **Thus the field calculation should be a minor part of even a full 3D simulation, in stark contrast to methods proceeding in the time domain (with Lienard-Wiechert formulas or retarded potentials).**

The plan for a self-consistent calculation based on macro-particles, say for CSR in a

chicane, is as follows:

1. Given the phase-space coordinates of N particles at $s = s_0$, construct smooth charge and current densities $\rho(\mathbf{r}, s_0),\ \mathbf{J}(\mathbf{r}, s_0),\ \mathbf{r} = (x, y, z)$.

2. Perform Fourier transforms to get $\hat{\rho}(x, \alpha_p, k)$, $\hat{\mathbf{J}}(x, \alpha_p, k)$.

3. Integrate the equations (1) for some interval Δs by an implicit rule, assuming the sources to be constant over that interval. Form all necessary components of the EM fields from $\hat{E}_y(s_0 + \Delta_s),\ \hat{H}_y(s_0 + \Delta s)$.

4. Perform inverse Fourier transforms to get fields as functions of $\mathbf{r}$, and use them to push particles to $s_0 + \Delta s$ with the full Lorentz force.

5. Return to step 1 with $s_0 \to s_0 + \Delta s$.

At step (1.) we need initial values for $\hat{E}_y$ and $\hat{H}_y$. Reasonable values for these would be the values they would have in an infinite straight wave guide excited by the given initial source, assuming it constant in s. There is an analytic formula for these fields. I suspect that most investigators would merely take zero for the initial fields.

To assess the cost of this algorithm I have verified the following: (a) the Fourier transforms in (2) and (3) take tens of milliseconds to perform and are not a source of error. The formation of all field components as mentioned in (3) is also trivial in cost. (b) using kernel smoothing [7] I find that a smooth 3D charge density $\rho(x, y, z)$ from 10^6 particles can be obtained in 3.8 seconds, while a 2D density $\rho(x, z)$, probably adequate for CSR in most cases, requires only 0.17 seconds.

As reported in the previous section, the field solver will take less than 2 seconds, going through one bend of a chicane in 300 steps. **Thus the only significant cost can come from particle pushing.** That will depend on the number of particles and the frequency with which it must be done. This frequency of updates depends mostly on the beam current, the bunch spectrum, and the bending radius.

I have not yet programmed particle pushing, but I am optimistic that the cost will not be excessive. At worst, this step could require a simple parallel program. One should take care to adopt an efficient symplectic algorithm.

VI. REMARKS ON SMOOTHING OF PARTICLE DISTRIBUTIONS

The world of particle simulations and PIC codes seems devoted to a restricted set of algorithms to smooth the particle distribution, in place for decades. For instance, one does particle deposition on a mesh, followed by a Fourier transform, filtering of that transform by a high frequency cut-off, then an inverse Fourier transform. A more direct approach with aesthetic appeal is to convolve the particle distribution with a smooth kernel of small support, which has unit integral [7]. With appropriate bookkeeping to tag all the particles within reach of the kernel on each cell in phase space, this becomes a very fast algorithm, as was mentioned above. Moreover, the result is "close to unique", by which I mean that there is low sensitivity to the type of the kernel if its reach (support) is in an appropriate range.

A still better method, if possibly more costly, might be the method of moving least squares, in which one gets a best fit in a certain sense as well as global smoothness determined by the weight function of the least squares [8]. Because of the approximative aspect, neglected in kernel smoothing, the result should be closer to unique.

Since smoothing is such an important part of simulations, I feel that a more careful and systematic study of the topic is in order. For this we should learn from the sophisticated efforts of statisticians [7] and numerical analysts [8].

VII. DIRECT SOLUTION OF THE VLASOV EQUATION VERSUS MACRO-PARTICLE SIMULATION

An approach in which smoothing is automatic and less ambiguous is based on direct solution of the Vlasov equation by the method of local chacteristics, also called the semi-Lagrangian method [9]. Although this has seemed to be too expensive in 6D phase space, or even in 4D for some problems, I now believe that time has come to make it competitive to particle methods. For similar resolution, in the sense that the number of macro-particles is equal to the number of grid cells in a Vlasov solution, the extra cost of Vlasov is in the interpolation step which updates the distribution function by evaluating the current distribution at grid points mapped backwards, thus at off-grid points. By a thresholding method in which updates are avoided when the distribution is negligibly small, this cost is reduced, markedly so in higher dimensions.

I am convinced that for single-pass systems, such as successive chicanes in a linear accelerator, a Vlasov treatment of CSR and space charge is entirely feasible in 4D, with modest equipment. I will not speculate about the cost of 6D, or the requirements for treatments of storage rings, but there is no reason to doubt success in an HPC environment.

VIII. BEYOND THE PARAXIAL APPROXIMATION TO THE FULL MAXWELL SYSTEM: JUST DO IMPLICIT INTEGRATION!!

At first sight it might seem that one could restore the second derivative $\partial^2/\partial s^2$ that was dropped in the derivation of (1). One would only have to write the system in first order form and proceed as before. This turns out to be a grossly unstable system, that cannot be integrated with any reasonable integration step, **if the integrator is explicit**. On the other hand, I fortunately noticed a paper from LBNL on laser plasma acceleration, which mentioned a so-called Crank-Nicolson method that contained a second derivative, unlike the standard Crank-Nicolson [10]

I wasted no time in trying this out in the CSR problem, and found that **Crank-Nicolson including the second derivative is stable if the step size is sufficiently large!** And "large" was just the value I was using anyway, as mentioned above.

I have seen nothing of the sort in the literature of differential equations or wave guides, and think it might be a new observation that deserves a closer analysis. I hope to pursue this with the help of mathematical colleagues. For us it means that we might treat corrugations in the vacuum chamber, which cause backward waves not allowed in the paraxial approximation. There might also be wide-ranging applications in wave guide theory, including optical wave guides and nano structures.

IX. THE EDUCATIONAL ANGLE

As was emphasized in charges to the GARD workshops, the education of new participants in accelerator physics is an important task. I think that development of the program I have outlined would be a very good Ph.D. thesis topic, especially for a student and professor with an interest in numerical analysis as well as physics. There is an opportunity to explore a new aspect of differential equations and new angles in smoothing algorithms, while also producing

a very useful practical tool. Through integration of the code in a general accelerator code tool box, the student would also learn a lot about the general problems of accelerator simulation, and would be well on the way to a career in that field.

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