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An ESME Update
(v. 7.2)

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Abstract

The program ESME for modeling the longitudinal degree of freedom of beam dynamics in proton synchrotrons was described in considerable detail in "User's Guide to ESME v. 7.1"[1] distributed about a year ago. This note corrects minor errors and omissions in the User's Guide, discusses bugs and crochets, notes fixes, and reports a few enhancements. Current work and plans are sketched. This note should be adequate to update the User's Guide.

Introduction

The program ESME has seen substantial use in the year since the major revision (v. 7.1) was described.[1] Users in general apparently have had few problems, but glitches have been found in the code and documentation.[1] Two of these could result in wrong answers; neither affected calculations using standard defaults. The options affected were time domain calculation of beam driven resonator and nonlinear momentum terms in the difference equation. The later discussion should be adequate to asses the extent to which past calculations may have been compromised. The other errors resulted in some features failing to function under some conditions.

The User's Guide promised the appearance of a more full treatment of the difference equations for the phasespace mapping. It is now available[2] along with another note which considers the contribution of betatron acceleration.[3] The latter shows that equating the perturn ΔE to $eV(\phi)$ is correct not only for the synchronous particle but also for the relative motion of others within practical energy range. The only effect is a fictitious or renormalized synchronous phase.

The code should continue to see some development. Additions made recently are described. Possibilities for further development are mooted with no implication of obligation

[1] Discussions with Xiamping Lu, Qing Wang, and Jim Griffin were helpful in exposing some of these problems.

to follow them precisely. Criticism or further suggestions from users will receive interested consideration, but ESME development is neither a hobby nor an industry. Such changes as are made will likely be either directly in the course of the author's work or be very simple to implement. The following sections cover separately documentation changes, bug fixes, speed enhancement, and present intentions.

Documentation Changes — Additions and Corrections

The User's Guide was compiled over several months, and several people made use of the various drafts, so just a few errors seem to have survived into the TM-1650 version. There have been some changes, however, related to additions and fixes to the code. Those changes are also included in this section. Page references in the following are to TM-1650.

R Command, p 9

The quantities ALPHA1, ALPHA2, and ALPHA3

These quantities are incorrectly defined in the parameter table. The correct data items are the expansion coefficients for $\Delta R/R$. The correct definition is also contrary to that given by the author in a recent MI note.[4] The corrected lines in the table should read as follows:

Variable	Default Value	Default Unit	Description
ALPHA1	None	-	Coefficient of $(\Delta p/p)^2$ in series expansion for $\Delta R/R$ about reference orbit.
ALPHA2	None	-	Coefficient of $(\Delta p/p)^3$ in series expansion for $\Delta R/R$ about reference orbit.
ALPHA3	None	-	Coefficient of $(\Delta p/p)^4$ in series expansion for $\Delta R/R$ about reference orbit.

FRAC parameter

In the table of parameters there is a typographical error on the range of the variable ϑ as set by the FRAC parameter. The entry should read

Variable	Default Value	Default Unit	Description
FRAC	1	-	Determines azimuthal periodicity, calculation restricted to $-180°/\mathrm{FRAC} \leq \vartheta \leq 180°/\mathrm{FRAC}$.

A Command, p 12

The description of the parameters VMATCHI and VMATCHF are replaced by the following description of VMATCH. This change is caused by a fix in the bucket-to-bunch matching feature described later.

Variable	Default Value	Default Unit	Description
VMATCHI(1:10)	F	-	For source I, VMATCH(I) = T results in the VI(I) being set so that source I is matched to the current distribution emittance.[a]

P Command, p14

Two distributions have been added, a matched elliptical distribution[5] and a distribution uniform between specified limits in ϑ and parabolic in E. The former is significant because it is the only distribution provided that is "microscopically" matched to the potential, *i.e.* having particle density distributed according to a function of the Hamiltonian. The way it has been implemented is adaptable to some other fully matched distributions. The elliptical distribution, however, seems to be generally a good choice for proton synchrotrons; it has an interesting and perhaps useful feature that the threshold for microwave instability is the same everywhere along the bunch. Because the projections of an elliptical bunch are parabolic, the parabolic distribution is a good one for unbunched beam.

The distribution generated by KIND = 11 is described in the User's Guide as particles along flow lines just above and below the bucket. At one time the SEPTRIX subroutine served this function, but somewhere in the migration from computer to computer the person making the translation decided that it was supposed to do something else. At this time the code has been dummied out; the attempt to use it will halt execution.

The new entries for the **P** command parameter table (p 14) are

Variable	Default Value	Default Unit	Description
KIND	1	-	Chooses the type of distribution to be generated: 11-Particles just outside of bucket — NOT AVAILABLE 14-Matched elliptical distribution of NPOINT particles with bunch area SBNCH 15-NPOINT particles uniform between THMIN and THMAX and parabolic in energy between REMIN and REMAX

B Command, p 24

There is a missing entry in the parameter table. NBRES gives the number of azimuthal slices of the ϑ region $-180°/\mathrm{FRAC} \leq \vartheta \leq 180°/\mathrm{FRAC}$ which become the intervals for the time domain calculation. The present default NBRES $= 10^4$ is not especially low; one may be able to save some computing time by giving a lower value in the $SCHG namelist input. The missing entry should read

	Default		
Variable	Value	Unit	Description
NBRES	10000	-	Number of time intervals in calculation of beam-induced on LCR resonator

Bug Fixes

The fixes described below have been introduced into the public source library on the Accelerator Division VAX (ALMOND::USR$DISK4:[ESME_FILES.CMSLIB03]) and the executeables called by the RESMEVAX and RESMEFPS commands on (or about) the various dates indicated. This note is the first formal documentation of the changes; the remarks in the CMS history in the source library have provided an interim record. All changes have been tested in some calculations, but there is no guarantee against iatrogenic disorders.

Nonlinear Momentum terms in the basic map

The essential nucleus of ESME is a nonlinear turn-by-turn map consisting of an energy increment difference equation and a phase slip difference equation. The relative phase slip of particle i is given by the ratio of the angular velocity of the synchronous particle to particle i:

$$S_i = \frac{\Omega_s}{\Omega_i} = \frac{\beta_s R_i}{\beta_i R_s} \quad . \tag{1}$$

Both of these trajectories may be distinct from the reference trajectory of mean radius R_c. The two particles then have momenta p_i and p_s different from the momentum p_c of a particle which follows the reference trajectory. For each particle $R(p)$ can be expanded about $R_c = R(p_c)$ in powers of $\delta = (p - p_c)/p$:

$$R(p) = R_c(1 + \alpha_c\delta - \alpha_1\delta^2 - \alpha_3\delta^3 + \cdots) \quad . \tag{2}$$

The discussion of the "phase slip factor" S in any of the references [2], [3], or [6] shows that the difference equation is in fact derived in this manner. The data items ALPHA1, ALPHA2, and ALPHA3 are just these momentum expansion coefficients of the path length. The quantity α_p is used to evaluate η and for some other auxiliary calculations, but the map has not been based on it since the extension of the code from first order momentum

dependence over ten years ago. In v. 7.2 the map is written almost directly with the form eq. 1.

However, the User's Guide gives states that the ALPHAn parameters are expansion coefficients of the momentum compaction α_p. The history of this error is long and mixed: at certain stages the code contained elements based on both definitions of the α_i. Practically speaking, as one can see by expanding α_p to first order,

$$\alpha_p = \frac{p}{R}\frac{\partial R}{\partial p} \approx \alpha_0 + (\alpha_0 + 2\alpha_1 \quad \alpha_0^2)\delta \ , \tag{3}$$

the result of using the expansion coefficients of α_p is to replace α_1 by the quantity in parentheses; the result will usually be too large because generally α_1 is positive. The effect is an exaggeration of the "Johnsen effect"[7] in transition crossing; away from transition or for small bunches crossing transition, there are no detectable effects. Note that the default value of ALFA1 is zero; therefore there would be no problems with calculations which were not explicitly concerned with this subject. The misstatement of the User's Guide was repeated by the author in a recent MI note[4]. This is probably as good a place as any to apologize to any who have been misled in transition crossing studies; my face is red.[2]

Time domain solution for high-Q resonator

For a short time after the User's Guide was issued there was an error in the time domain model of a high-Q resonator giving the wrong result for the excitation arising from prior turns. The solution is constructed by convolution of the current distribution with a single turn Green's function; the contribution of prior turns is included by taking initial conditions reflecting the state of excitation at the end of the previous turn. The quantities that are carried over from one turn to the next are just the final voltage and its time derivative. The derivative was being evaluated numerically by first order difference between last and next-to-last time slices. The difference is subject to large error because of statistical fluctuation of bin population. Furthermore, there was a sign error so that the result was wrong by 180° in phase. However, the Green's function solution also gives an analytic result for the derivative. The code has been changed to use the analytic expression for the derivative so that it is now evaluated from the entire distribution. This change was made in the public source library by May 1990. The affected subroutine is HIQRES, and only calculations invoking the time domain model by setting the QREZON parameter to .TRUE. in the $SCHG namelist could be compromised. Although coupled bunch instability results seem to have been at least qualitatively correct, the details of beam loading were clearly wrong.

[2] The question of the definition of α_1 was originally raised by Bill Ng in September, 1990. Although I did not correctly react to the question at the time, it was because of his query that the problem was diagnosed when the effects showed up in my own work.

Excessive time in the CONTOUR subroutine

Even when no contour was to be plotted, the routine DISPLAY in v. 7.1 called BUCKIT to get the bucket area and height for the phasespace plot caption block. This routine calls CONTOUR to generate a closed bucket contour from the difference equations. Near transition energy, where the standard bucket disappears, BUCKIT and CONTOUR could try for several minutes to find a closed contour before giving up. The problem has been addressed by using the standard bucket area and height formulae to evaluate these quantities unless a bucket contour has been requested in the $GRAPH namelist input. Furthermore, the response of BUCKIT to a failure of CONTOUR has been changed from a reduction of the interval of numerical integration to moving the starting point for the contour slightly farther away from the estimated location of the unstable fixed point. BUCKIT makes three tries to close the contour; each retry moves the starting point closer by DELCON to the calculated location of the stable fixed point, where DELCON is the precision parameter which can be read in with the $GRAPH namelist input. The default value is 0.01. The previous strategy of going to a finer integration interval rarely succeeded and progressively increased the execution time each try. The use of the formula values in the phasespace plot caption can be misleading in some circumstances because they are wrong for multiple rf systems or too close to transition. However, during recent work on transition crossing literally hours of computer time have gone toward calculating contours that were not requested explicitly by the input parameters. In fine, if one wants to know the bucket area and height by numerical integration of the difference equations close to the separatrix, one must explicitly request the plotting of a bucket contour. Corrections have been installed in DISPLAY and BUCKIT during January 1991.

Failure of MATCH

By setting one or more of the switches VMATCHI(1:10), VMATCHF(1:10) to .TRUE. with the $RF namelist input, one was supposed to get respectively an initial or final voltage for which the indicated source acting by itself would provide a bucket matched to the existing phasespace distribution. The code provided in v. 7.1 does not perform this function under any conditions and results in a program abnormal termination on arithmetic exception. The chosen fix is simultaneously an enhancement and a restriction of the features described in TM-1650. The v. 7.1 code has been entirely replaced. The new algorithm establishes an estimate of the matching conditions by finding the bucket resulting in $\beta_{\rm long}$ (longitudinal analog of the Courant-Snyder lattice function) equal to that implied by the ratio of bunch height to bunch width and the assumption of no tilt. This is called a linear match because it is based on the properties of the first order linear differential equations describing the synchrotron motion. Using the linear result to set the scale, a contour of area somewhat less than the bunch area is constructed for a trial series of different rf voltage - synchronous

phase pairs. The voltage resulting in the smallest fraction of the distribution outside of the contour is found by second order interpolation on the results of the trial series. This voltage is returned as VI(I) and the corresponding synchronous phase as PSII(I). The new code is an enhancement because the non-linear search gives better results where the distribution is not close to the Hamiltonian flow for any value of the voltage of system I. If the nonlinear search fails to find a minimum in excluded phasespace points, the result of the linear match is returned. The present version has a single array of logical switches VMATCH to select the rf systems for which a matched voltage and phase are desired. The results are always returned as the initial values because this is the only way the feature has ever been used in practice. The possibility of moving these values into VF(I) and PSIF(I) by a SHAZAM routine provides for the unlikely event that a user may wish to evolve the voltage to a matched value from some other starting point. This does, however, represent an apparent reduction in function from that specified in TM-1650. The fix was installed 23 January 1991.

Synchronous phase for waveforms with PSI(I) $\neq$ 0

The use of the the automatic calculation of synchronous phase (ISYNC = 1 parameter option in SRF namelist) along with non-zero values for the rf phases PSI(I) has resulted in conflicts where the energy gain per turn was not what was expected. The problem has been fixed so that, as always intended, PHIS gives the amount that a waveform, including effects of any explicit phases, must be shifted to produce the requested $\dot{p}$. If the PSI(I) give the correct energy gain, PHIS will be exactly zero. If they give approximately the requested energy gain, PHIS will be a small correction. In a typical case with a one rf source having PSI(1) = 0, H(1)$\times$PHIS is exactly the conventional synchronous phase angle. The programming required to interpret all reasonable combinations of PSI, PDOT, V, ISYNC, *etc.* is a bit elaborate; the possibility has not been entirely excluded that what seems reasonable to some user may produce unexpected results. The last changes to the source related to these problems were made in August 1990.

Failure to close decelerating bucket contours

The CONTOUR routine was failing to find the bucket boundary for decelerating buckets. This was a nuisance level problem which was ignored until the cause was spotted while working on synchronization. The fix was not made until January 91. The error was not in the contouring routine itself, but rather in the value for the expected unstable fixed point calculated by LINBKT.

Faster Difference Equations

In v. 7.1 the effect of setting the **A** command parameter LGRTHM equal to 2 was to provide difference equations linear in everything except terms from the potential. The purpose of this option was to provide a test of the approximation for particular input data; it was not designed to realize a gain in computing speed, however. The code now has been streamlined to realize most of the saving from the simpler difference equations without having to substitute a new FOLLOW subroutine in place of the standard one. There is no change to the input or results. For most applications where the energy does not come close to the transition energy and the particles of interest remain near the synchronous particle, the simple difference equations are entirely adequate, and they may save 30% of the execution time, more or less depending on active options.

Plans and Projects

ESME has been combined with at least four different graphics packages since its earliest incarnation in the '70's; the current version uses DI3000[8] plus its GRAFMAKER higher level interface. These products, though commercially available, are not widely used at high energy physics or accelerator laboratories. It is a high priority to find a system with adequate capabilities that is in reasonably wide use and has reasonable prospects of longevity. Because the demands of ESME are modest, the capability question is primarily that of a simple user interface for line plotting, scatter plotting, and histograms with pleasing legends and labels. The questions of availability and longevity have always been the tough ones. For an earlier effort to make the code available at CERN, GD3 was adopted because it had pleasing features and because both Fermilab and CERN seemed committed to support it. The current thought is to adopt HIGZ for the same reasons. Perhaps this choice will be more fortunate because HIGZ is a somewhat higher level interface to GKS. GKS itself shows signs of becoming a fairly widespread standard. Fermilab has additionally developed HIGZ as an interface to DI3000 and may be edging toward a policy of interfacing it to any other system it may adopt in place of DI3000 for general use. Therefore, although it is not a standard commercial product, HIGZ should be available from the largest high energy physics laboratories for a considerable time into the future. It is written in FORTRAN, available essentially without restriction, and, one hopes, easily portable. Redoing the graphics will surely result in some changes in appearance but probably little in the way of altered function.

Efforts to get a production version and development capability installed on a SUN workstation are just getting started. Because ESME has already been used on SUN's there may be no big problems. However, verification that output is precisely the same as that from VAX and Amdahl versions will probably be slow to come because there will be no systematic validation effort.

It is likely that the distribution of particles just outside of the bucket will be reactivated soon because it should require a straightforward return to old code.

Conclusion

The description of ESME given in the User's Guide for v. 7.1 (TM-1650) remains generally correct at v. 7.2 (6 February 91). An omission from and a correction to the guide have been noted. Furthermore, an addition related to new starting distribution options and a change corresponding to a reworked bunch matching capability have been reported. Making small changes to TM-1650 at the indicated places will render the documentation current and as complete as available.

There have been few complaints about bugs from general users, but one should assume there are yet traps for the unwary. All that are known now are corrected or, at least have been worked on, at v. 7.2. Unless the graphics rework results in important changes, a direct revision of the User's Guide is not foreseen.

References

[1] S. Stahl and J. MacLachlan, "User's Guide to ESME v. 7.1", Fermilab internal note TM-1650 (26 February 90)

[2] J. A. MacLachlan, "Difference Equations for Longitudinal Motion in a Synchrotron", Fermilab note FN-529 (15 December 89)

[3] J. A. MacLachlan, "Differential Equations for Longitudinal Motion in a Synchrotron", Fermilab note FN-532 (25 January 90)

[4] J. MacLachlan, K. Y. Ng, S. Peggs, "The Definition of α_1: Circumference, Johnsen, or ESME?", Fermilab Main Injector internal note MI-0038 (October 1990)

[5] A. Hofmann and F. Pedersen, "Bunches with Local Elliptic Energy Distributions", IEEE Trans. Nucl. Sci., **NS-26**, No. 3 (June 79), pp 3526–3528

[6] J. A. MacLachlan, "Fundamentals of Particle Tracking for the Longitudinal Projection of Beam Phasespace in Synchrotrons", Fermilab note FN-481 (15 April 88)

[7] K. Johnsen, in "Proc. of the CERN Symposium on High Energy Accelerators" vol. 1 (1956), p106

[8] DI3000 and GRAFMAKER are products of Precision Visuals, Inc.