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MURA-717

WRITE-UP OF MURA 704 PROGRAM F51

PARTICLE SPACE-CHARGE PROGRAM

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(Revised by F. J. Kriegler August 1964)

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EPITOME

As an approach to solving the problems of nonlinear longitudinal space-charge effects and of space-charge effects in the presence of radio-frequency fields, this IBM 704 computer program performs a linear integration of the equation

$$\ddot{\phi} = -(\Gamma - S \sin \phi) - E(\phi, t)$$

for as many as 10,000 pairs of initial conditions (particles) ϕ, $\dot{\phi}$; the space-charge field E being computed by convolution of a space-charge kernel and the particle density obtained by scanning the banks of ϕ at the beginning of the current time step.

The initial values are specified by giving a density $\sigma(\phi, \dot{\phi})$ of particles at time zero.

The output is in the form of tables of ϕ, $\dot{\phi}$ for selected particles, tables of the density and space-charge field as functions of ϕ, plots of $\rho(\phi)$, plots of $\sigma(\phi, \dot{\phi})$, and plots of trajectories of selected particles in the $(\phi, \dot{\phi})$ phase space.

METHOD

If $Y = -\dot{\phi}\,\Delta t/2\pi$ and $X = \phi/2\pi$, then $\dot{X} = -Y/\Delta t$,

$\dot{Y} = (\Delta t/2\pi)\left[\Gamma - \sin 2\pi X + E(2\pi X, t)\right]$; Δt = time step duration.

Two integration schemes are available. The first is quicker but less accurate.

It may be derived from generating functions according to Hamiltonian mechanics, so that it preserves density in phase space except for round-off error. The stepping equations are

$$X(t + \Delta t) = X(t) - Y(t)$$

$$Y(t + \Delta t) = Y(t) + \left[(\Delta t)^2/2\pi\right] \left\{\Gamma - \sin\left[2\pi X(t + \Delta t)\right] + E\left[2\pi X(t + \Delta t), t\right]\right\}$$

for each particle.

The second scheme is similar save that the argument in the sine term is $\frac{1}{2}\left[X(t) + X(t + \Delta t)\right]$ and the space-charge term in $\dot{Y}$ is taken as the average of E between X(t) and X (t + Δt) for each particle. This probably is not a canonical scheme.

These options are obtained by calling for F51 decks S or V respectively when a run is submitted.

Note that sin (2π X) is approximated by the function $(X/|X|)\left[1 - (4|X| - 1)^2\right]$, X being carried "modulo" 1 such that it lies between $-\frac{1}{2}$ and $+\frac{1}{2}$.

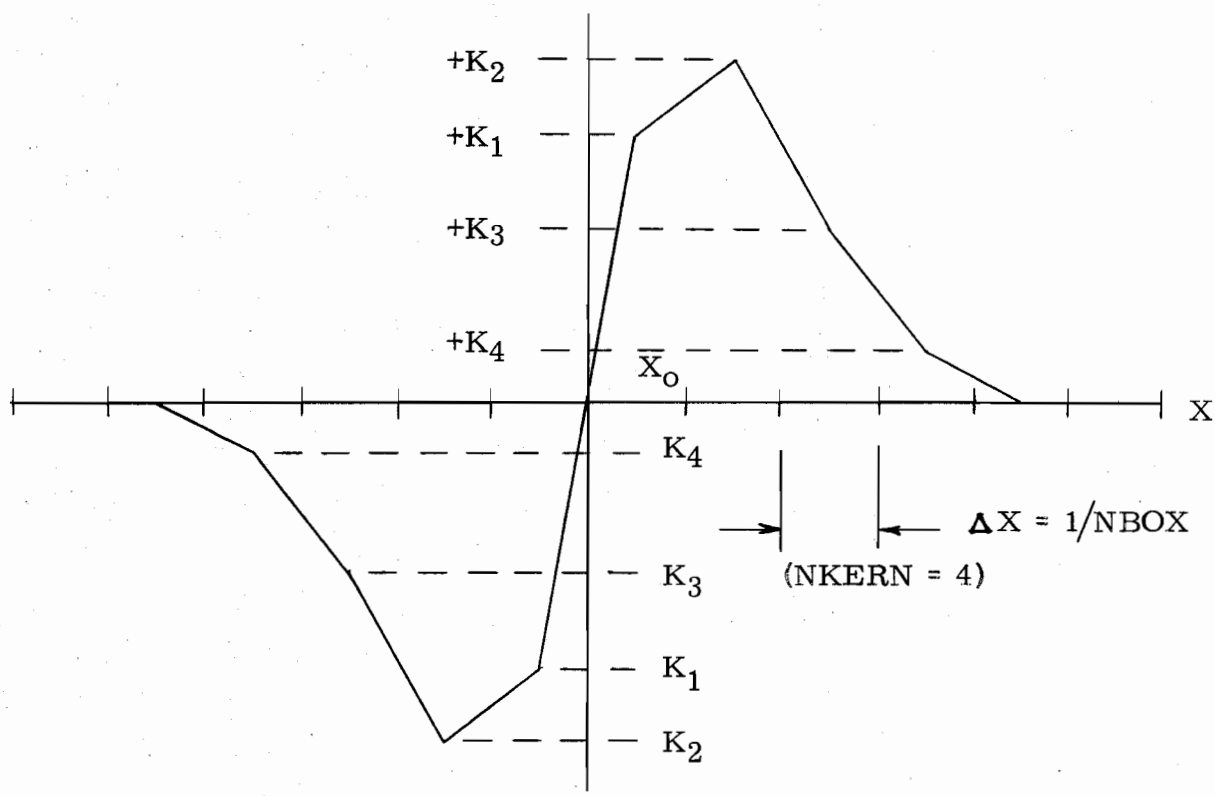
For calculating speed $(\Delta t)^2/2\pi$ is taken as an integer LNTAU power of 2 : $(\Delta t)^2/2\pi = 2^{-\mathrm{LNTAU}}$. The space-charge field is taken as a function piecewise linear on the interval $X \in (-\frac{1}{2}, \frac{1}{2})$ of periodicity 1, being specified at NBOX equidistant values of X. (NBOX is an integer power LN2BOX of 2.) A step function density is found by assigning to each particle a characteristic width of 1/NBOX and dividing this width in a linear fashion between the two density boxes spanned by this width. The density is then given by NBOX numbers which add to yield the total number of particles. This density is convoluted with a kernel K_j, j = 1 to NKERN to give the field as a step

function in X:

$$E_j = \sum_{n=1}^{NKERN} K_n \cdot (\rho_{j+n} - \rho_{j-n}) \text{ with } \rho_m = \rho_{m+NBOX}$$

K_j is negative for a physically real situation. When used to find E(X), a linear interpolation is performed on the values E_j.

The result of all this is best seen as an effective field kernel defined as the contribution of a particle at X_o to the field at X (see graph).



This function is actually a linear interpolation between the values of the kernel specified.

$$K_j \text{ is } Z_{100+j} \qquad \text{for} \qquad j = 1 \text{ to NKERN} \leq 32$$

on the agendum sheets.

Provision is made to omit calculation of the space-charge field: set IFIELD = integer < 0 ; and to omit calculation of the rf term

$\sin(2\pi X)$ in the motion equation: set IRF = integer < 0.

For purposes of following the net motion with a few numbers, as many as 200 test particles may be carried. These differ from regular particles only in that they do not contribute to the density. NTEST such particles are so carried.

Test particles are entered by specifying X, Y at t = 0, with $X_i = Z_{i+150}$, $Y_i = Y_{i+151}$ for i = 1 to NTEST.

Regular particles are entered as follows: The function

$$F = Z_{30} + Z_{31} U + Z_{32} U^2 + Z_{33} \cos\left[2\pi (Z_{35} U + Z_{36})\right] + Z_{41} V + Z_{42} V^2 + Z_{43} V^3 + Z_{44} V^4$$

with $U = Z_{25} X_o + Z_{26}$ and $V = Z_{27} Y_o + Z_{28}$ is evaluated on a rectangular I_x by J_y mesh beginning at $X = 1/2\, I_x$, $Y = Y_o + \frac{\Delta Y}{2}$ and ending at $X = 1 + 1/2\, I_x$ and $Y = Y_o + (J_y - 1)\,\Delta Y + \Delta Y/2$. If Z_8 is negative, $[F]$ particles are entered in the rectangle in X, Y space about the point X_o, Y_o. $[F]$ is the integer part of F if $F \geqslant 0$. If Z_8 is plus or zero, the number F is compared to a set of NVAL pairs of limit values (Z_{301}, Z_{303}), (Z_{304}, Z_{306}), $\cdots$; if F lies in the closed interval (Z_{301}, Z_{303}), then Z_{302} particles are entered in the rectangle about X_o and Y_o. If Z_5 is negative, these particles are scattered randomly in the rectangle of sides $1/I_x$ and ΔY centered about the mesh point X_o, Y_o for which F was evaluated. Z_6, a positive power of 2, determines which of fifteen possible "random" sets of numbers are used. In a series run the set used for each run is different whether or not Z_6 is different. If TRIGF is nonzero, then F is not evaluated. Rather, a density of sinusoidal variation is generated: particles

are placed on J_y lines of fixed $Y = (J - 1)\Delta Y + Y_o$ for $J = 1$ to J_y with sinusoidally varying spacing. A density $Z_{45} + Z_{46} \cos\left[2\pi(Z_{47} + Z_{48} X)\right] + Z_{50} \cos\left[2\pi(Z_{51} + Z_{52} X)\right]$ is thereby generated, $Z_{45} J_y$ being the total number of particles entered. This function should not be $\lesssim 10$. If $Z_5 \leq -1$, the particles are placed randomly in the interval between them, the random number again being generated from Z_6. INDX is the total number of particles, NTEST + NREGULAR. Particles are indexed as follows: X_1 through X_{NTEST} are test particles, and $X_{1+NTEST}$ through X_{INDX} are regular particles.

Other control numbers: ID is an integer between -32767 and 32767. NZ is the number of input floating point numbers (Z_j, $j = 1$, NZ) to be printed out before the run. YLIMIT is the maximum allowable value of $|Y|$ for all particles. When this is exceeded, all the Y's are halved and this test is redone. Δt is reduced by the factor $1/\sqrt{2}$ and plot parameters changed accordingly. The statement "****** DT HALVED AFTER STEP -- NØ. XX ···" is printed each time this is done. XX is a count of the number of time step changes. The octal form of LNTAU is printed. The test for exceeding YLIMIT is performed every NCYCLE time steps.

Output-Control Numbers:

NAME	NUMBER OF CYCLES BETWEEN
NPLRXY	Plots of σ (X, Y)
NPRR	Prints of ρ (X)
NPLR	Plots of ρ (X)
NPRXY	Prints of X, Y for test particles
NPLXY	Entries of test particle phase points into the trajectory plot

A cycle contains NCYCLE time steps.

The vertical limits for the ρ plot are zero and MAXIMUM ($\rho_{NOMINAL}$, ρ_1, ρ_2, $\cdots$, ρ_{NBOX}). Those for the σ plot are Y_σ^{MAX} and Y_σ^{MIN} unless there is a nonzero value of σ for $|Y| > Y_\sigma^{MAX}$ in which case they are $\pm|\text{MAXIMUM}\ (|Y_i|)|$. If Z_{142} is $\neq 0$, then this self-adjusting feature is not used and the number of particles above and below the picture is printed. The picture consists of an array of 60 X 40 integers giving the number, if not zero, of particles in the appropriate rectangle in (X, Y) space. Y_σ^{MAX} and Y_σ^{MIN} are scaled during time step changes.

The vertical limits for the trajectory plots are Y_{TRAJ}^{MAX} and Y_{TRAJ}^{MIN} which are scaled at time step changes. These plots assign a symbol A, B, $\cdots$, Y, Z, 1, 2, $\cdots$, 8, 9, +, /, ·, $, , , =, (,), or - to each of up to 44 particles whose coordinates are X_j, Y_j for $j = I_{TPLOT}^{MIN}$ to I_{TPLOT}^{MAX} and at each entry stores the X_j's and Y_j's by storing the appropriate letter in an image of the output page. If two different particles fall at the same point within a resolution of 100 by 60 points, an asterisk is stored instead of either particle symbol. At the end of run this page is printed. Points falling off the plot are ignored.

A total of NTOTAL time steps are taken.

When test particle coordinates are called, X_i and Y_i are printed for $i = N_{PRINT}^{MIN}$ to N_{PRINT}^{MAX}.

If NDUMP is a positive integer, all data from a run are written on Tape 2 every NDUMP cycles. The run may be continued at any later time with new control parameters by putting this tape on unit 3, raising switch 3 and reading in the program, a control card, and the new data. The control card contains the run number in Columns 1 through 6 in integer form, right adjusted, the step count in Columns 7 through 12 and a new value of LNTAU

in 13 through 18. If the new LNTAU is zero, nothing is changed; if nonzero, all Y's, plotting parameters, Δt, etc. are scaled accordingly. When such a dump is made, a note is made on the output. The tape for this type of dump must be especially prepared. This is done by putting a scratch tape on unit 2 and following instructions printed on line. Thereafter the tape may be used for as many such dumps as will fit on it. Various remarks are printed on line if tape errors occur, the run called for is not found, the dump tape is full, etc. These may be self-explanatory.

Progress of a run may be determined while running by raising switch 4. A run may be abandoned by raising switch 6 and following printed instructions. A run may be interrupted by raising switch 1 and providing a scratch tape on unit 1. The entire status of the machine is then stored on the tape and may later be continued by loading from Tape 1 (cf. MUSAVE, MURA-562).

All significant output is off line to be processed using MURA X-25 on the 1401. The output is mostly self-explanatory.

Data are read by MURCD2 (MURA-536). Use equivalent of agendum attached.

Series runs may be made.

A set of data for one run consists of at least one card containing an integer, the first END DATA card, at least one containing a fraction, and the second END DATA card. Three END DATA cards should follow the last data card.

On the agendum and the output the first group of numbers are integers IG_j for $j = 1, 77$; the second group are fractions Z_j for $j = 1, 500$. The addresses on the agendum give the subscript, e.g., IG_1 is ID; Z_{80} is gamma.

ADDITION TO THE F-51 PROGRAM - - - - - - - - - - - - F. J. Kriegler

Modifications were made to the F-51 Program to accommodate the possibility of using a kernel function that is not antisymmetric as is the space-charge kernel. This resulted in a modification of subroutines INFELDS and OPUS IV. The kernel must be specified for NBOX points, the value NKERN must equal NBOX. To get the larger number of kernel values into the existing program the kernel is read into locations Z_{601} to $Z_{601+NKERN}$. A further modification was made to OPUS IV. Instead of YLIMIT being a test value for rescaling the Y's and Δt, any particle exceeding YLIMIT is assumed lost. The number of particles is then reduced by one.

A modification was made to the subroutine WORPRO. This modification results in a plot of $E(\phi, t)$ superimposed on $\rho(X)$ and an additional plot of $\sin\phi$ superimposed on $E(\phi, t) - \sin\phi$.

The relation of the computer variables X, Y to the real system variables is as follows:

$$X = h\left(\frac{\phi}{2\pi} - f_s\, t_{real}\right) \qquad f_s = \text{synchronous frequency}$$

$$Y = -\sqrt{\frac{h\, f_s'}{2\pi\, e\, V_g\, f_s}}\,(E - E_s) \qquad f_s' = \left.\frac{df}{dE}\right|_{f_s}$$

$$t_{comp} = \sqrt{2\pi\, h\, e\, V_g\, f_s\, f'}\; t_{real}$$

$$\mathcal{E}_{comp} = -\frac{2\pi R}{V}\,\mathcal{E}_{real}$$

$$\text{Kernel}_{comp} = -\frac{2\pi R\, e\, N}{Vn}\,\text{Kernel}_{real}$$

N = number real particles

n = number of macro-particles

MURA/FORTRAN AGENDUM

PROGRAM NO. F51 SUBMITTER _____

Instructions:

1. Enter Program number and submitter's name above.
2. Enter address and value below for parameters desired.
3. Enter sense switch settings: _____ _____ _____ _____ _____ _____

Notes:

1. Decimal points may be omitted only if understood to follow the rightmost digit.
2. Addresses may not contain more than 4 digits.
3. Factors may not contain more than 8 digits.
4. Exponents may not contain more than 2 digits.
5. Exponents may be omitted if zero. If not, they must be signed.

Parameters	Address	Value	Parameter	Address	Value
ID	1		N^{MIN}_{PRINT}	58	
NZ	19		N^{MAX}_{PRINT}	57	
IFIELD	23				END DATA
IRF	34		RANDOM SWITCH	5	
NPRXY	20		RANDOM GENERATOR	6	(1)
NPRR	25		TRIGF	7	
NPLR	26		F = NO	8	
NPLXY	27		Z_9	9	
NPRXY	28		I_X	21	(1)
NDUMP	50		J_Y	22	(1)
NCYCLES	35		ΔY	23	
NTOTAL	29		Y_o	24	
LN2BOX	30		Z_{25}	25	(1)
LNTAU	32		Z_{26}	26	
NKERN	33		Z_{27}	27	(1)
I^{MIN}_{TPLOT}	4		Z_{28}	28	
I^{MAX}_{TPLOT}	5				

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Parameter	Address	Value	Parameter	Address	Value
NVAL	29		Z_{51}	51	
Z_{30}	30		Z_{52}	52	
Z_{31}	31		GAMMA	80	
Z_{32}	32		Z_{84} minus below transition	84	(1)
Z_{33}	33		$\rho_{NOMINAL}$	87	
Z_{34}	34		YLIMIT	90	
Z_{35}	35		K_1	101	
Z_{36}	36		K_2	102	
Z_{41}	41		K_3	103	
Z_{42}	42		K_4	104	
Z_{43}	43		K_5	105	
Z_{44}	44		...		
Z_{45}	45		$Y_{\sigma MAX}$	140	
Z_{46}	46		$Y_{\sigma MIN}$	141	
Z_{47}	47		Y^{MAX}_{TRAJ}	143	
Z_{48}	48		Y^{MIN}_{TRAJ}	144	
Z_{50}	50				

MURA/FORTRAN AGENDUM

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Parameter	Address	Value	Parameter	Address	Value
NTEST	150			167	
X_1^{TEST}	151			168	
Y_1^{TEST}	152			169	
X_2^{TEST}	153			170	
Y_2^{TEST}	154			171	
X_3^{TEST}	155			172	
Y_3^{TEST}	156			173	
...	157			174	
	158			175	
	159			176	
	160			177	
	161			178	
	162			179	
	163			180	
	164			181	
	165			182	
	166				

MURA/FORTRAN AGENDUM

PROGRAM NO. F51 SUBMITTER _____

Instructions:

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Parameter	Address	Value	Parameter	Address	Value
F^{MIN}_{LIM1}	301			318	
N_1	302			319	
F^{MAX}_{LIM1}	303			320	
F^{MIN}_{LIM2}	304			321	
N_2	305			322	
F^{MAX}_{LIM2}	306			323	
F^{MIN}_{LIM3}	307			324	
N_3	308			325	
F^{MAX}_{LIM3}	309			326	
...	310			327	
	311			328	
	312			329	
	313			330	
	314		K_1	601	
	315		↓	↓	
	316		K_{128}	728	
	317				END DATA