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SNEER — A Digital Computer Program for the Simulation of Charged Particle Beams and Electrostatic Lenses

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SNEER--A DIGITAL COMPUTER PROGRAM FOR THE SIMULATION OF
CHARGED PARTICLE BEAMS AND ELECTROSTATIC LENSES

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ABSTRACT

A digital computer program for the simulation of charged particle beams in complex electrostatic lens systems is described. Poisson's Equation is solved on a large matrix to simulate the potentials in rectangular or axisymmetric configurations including dielectrics if needed. Relativistic trajectory computations are employed, including induced magnetic fields, to simulate beams or charged particles of any energy. The beam may be injected with any energy or spatial distribution, including point sources. The input data are described in detail and a sample data set is presented in the Appendices.

The program is intended to be an engineering tool which will produce results with an accuracy of one or two percent with modest effort in setting up the problem. Simulations on a CDC 660D typically require two minutes or less, and complete solutions including plots of trajectories and equipotentials are frequently obtained in less than 30 seconds. Results for some specific cases are shown to be within two percent of experimental or exact analytical results.

Copies of the program will be available through the Argonne Code Center, Argonne National Laboratory.

NOTICE

SUMMARY

SNEER has been found to be a powerful tool for the analysis of charged particle beams and trajectories. Inclusion of relativistic trajectory computations and the ability to include dielectrics in the potential relaxation enables the program to handle virtually any type of beam configuration not including a source--such as a cathode.

Examples shown here have produced results within a few percent of exact theoretical and experimental results. In Appendix C, a sample input data set is presented for still another application of the program. Here, trapped electron orbits are traced in electric and magnetic fields in an ion gauge configuration.

INTRODUCTION

A digital computer program for the simulation of charged particle beams in complex electrostatic lens systems has been written. The programming techniques are similar to those reported earlier^{1,2} but are simplified and improved to permit very rapid solutions for lenses of complex shape. The program is intended to be a flexible engineering tool rather than a precise method of determining detailed lens properties, such as the program described by Natali, et al.³ Space-charge free solutions with charged particle trajectories can frequently be obtained in less than 30 seconds on a CDC 6600 digital computer. Solutions with significant space charge can generally be obtained in less than 10 minutes (typically less than two minutes), the time varying with the importance of the space charge and the complexity of the lens.

Relativistic trajectory computations are employed to permit the simulation of beams (or particles) of any energy. A large rectangular matrix is employed to simulate the potentials in axisymmetric or rectangular configurations and to permit accurate descriptions of fairly complex electrode and dielectric systems. The beam may be injected with any energy or spatial distribution, including point sources, but no cathode or other such source is included in the simulation.

The input data for the program are described in Appendix A and data sheets are shown in Appendix B. The sample data set is presented in Appendix C and a listing of the SNEERA program (with space-charge) is presented in Appendix D.

SIMULATION METHOD

The program is a combination of two older programs for the simulation of Poisson's¹ and Laplace's² equations. Improvements have been made in both the speed and accuracy of the computations. The simulation consists of alternately relaxing the potentials and computing trajectories (ions or electrons) until two consecutive sets of trajectories are the same. A general flow chart is shown in Fig. 1.

Fig. 1. General flow chart for SNEER.

The potentials are determined by iterative relaxation on a large matrix array employing Poisson's or Laplace's equations in difference form. Dielectrics may also be included in the simulation if needed. Over-relaxation is extensively employed to reduce the solution time for the potentials to generally less than 60 seconds and frequently to as little as two or three seconds on each cycle through the program.

The standard five-point relaxation formulas are employed, where for the general point

$$V_{i,j} = \frac{V_{i,j+1} + V_{i,j-1} + V_{i+1,j} + V_{i-1,j}}{4} + \frac{\Delta r}{8r_j} (V_{i,j+1} - V_{i,j-1}) - \rho_{i,j} \quad (1)$$

and for points on the axis

$$V_{i,j} = \frac{1}{5} (4 V_{i,j+1} + V_{i+1,j} + V_{i-1,j}) - \rho_{i,j} \quad (2)$$

where V is the normalized potential and i , j , and r_j are defined in Fig. 2. $\rho_{i,j}$ represents the normalized space-charge densities on a matrix identical to the V matrix. The space-charge densities are computed directly from the trajectories. Relaxation is carried out at each point by passing up each column across the matrix, and then by passing down each column backwards across the matrix; this permits corrections to propagate rapidly in all directions and helps reduce systematic errors.

Two forms of over-relaxation are employed. The equations are initially solved on only the odd-numbered points of the matrix. This permits corrections to propagate much more rapidly since only about a fourth of the points

are employed. The second over-relaxation is the more standard form of multiplying the residuals at each point from cycle to cycle by a constant, e.g.,

$$V_{n+1} = (V_{\text{new}} - V_n)\beta + V_n, \quad (3)$$

where V_{new} is computed from Eq. 1 or 2 and V_n is the voltage value from the n 'th cycle. β is usually set at 1.8 initially and is reduced to one as convergence is approached. Optimized values for β are described by Sheldon,⁴ but $\beta = 1.8$ has been found quite satisfactory.

Dielectric interfaces, if present, are computed by a method described by Dorny⁵ and described in some detail in Ref. 2.

Trajectories are computed using a solution of the relativistic Lagrangian

$$L = eV = e(\vec{A} \cdot \vec{v}) - m_0 c^2 \left(1 - \left(\frac{v}{c} \right)^2 \right)^{1/2}, \quad (4)$$

where e is the electronic charge, V the potential, $\vec{A}$ the magnetic vector potential, $\vec{v}$ the velocity, m_0 the rest mass, and c the velocity of light. Details of this solution, which include induced and applied magnetic field, have been described earlier.¹

Virtually any type of trajectory can be computed in space-charge-free solutions, but oscillatory trajectories should be avoided if space charge is employed. Space-charge densities are added to the adjacent points of the ρ matrix when the trajectories cross matrix rows or columns. Trajectories will terminate at the boundaries of the matrix, on electrodes or at specified dielectric surfaces. All induced effects, except the relativistic mass change, can be eliminated by specifying zero current, i.e., negligible space charge.

Accuracy of the computation is generally limited by the size of the matrix employed and the complexity of the lens being simulated. Results within one or two percent of theory or experiment can be obtained with modest care in setting up the problem (see Ref. 2). Examples are given below.

RESULTS

Excellent agreement has been obtained for cases where data can easily be compared. A comparison with the results of Natali, *et al.*³ and Kuyatt, *et al.*⁶ (Fig. 3) for a two tube electrostatic lens shows differences of less than one percent in potential and in focal properties. A comparison of typical potentials along the axis and the focal lengths of a 20 to 1 potential ratio lens is given in Table I.

Table I. Comparison of axial potentials and focal properties with those of Natali³-Kuyatt.⁶

$\frac{z}{D}$	$V(z)$	$V(z)$ Natali
0.0	0.50024	0.50000
0.05	0.43371	0.43453
0.10	0.36992	0.37140
0.20	0.25765	0.25953
0.50	0.07054	0.07090
1.0	0.00668	0.00659

Focal Properties $V_2/V_1 = 20$

	<u>Focus</u>	<u>Focus-Kuyatt</u>
F_1	1.192	1.199
F_2	0.623	0.632

Fig. 3. Trajectories for the two-tube electrostatic lens with a 20 to 1 potential ratio, compressed 4 to 1 in the axial dimension. A 0.1 D gap is used between cylinders, a la Natali, et al.³

The really big difference between the two solutions is the time required to obtain them. Natali³ required 16 minutes on an IBM 360 Mod 65 to obtain potentials needed to solve the problem. The program described here took 18 seconds. (on a CDC 6600) to relax the potentials for the complete lens, compute the trajectories and obtain plots of equipotentials (Fig. 4) and trajectories (Fig. 3). The results are not as accurate as Natali-Kuyatt but for most engineering purposes would be sufficient.

Fig. 4. Equipotentials for the two-tube electrostatic lens, a) the central part of the lens, b) compressed plot of complete lens, with equipotentials every 5% of maximum potential.

A more practical example is shown in Figs. 5 and 6. Here a lens described by Liebmann⁷ is shown with and without a screen across the entrance and exit planes. With the screens, the beam is well focused leaving the lens; and without the screen, there is significant distortion in the lens and the beam is divergent as it leaves the region of the lens.

It was desired to sample a high-energy ion beam and to measure its constituents in a time-of-flight spectrometer. This required the focusing of the point source at a target two meters from the lens. The computer program suggested a slightly longer (3.9%) focal length than that given by Liebmann⁷ and indeed better transmission was obtained by placing the beam source at this focus point.

Fig. 5. Electrostatic lens with 5% equipotentials (a) and trajectories from a point source (b).

Fig. 6. Equipotentials (a) and trajectories (b) for lens with screens across the entrance and exit planes.

Figure 7 shows a perveance 1.54×10^{-6} ampere (volt) $^{-3/2}$ electron beam in a drift tube. This corresponds to the maximum electron current that can be transmitted through a tube with a length-to-diameter ratio of 5.⁹ Increasing the current by one percent will cause interception before the end of the tube is reached.

The beam is injected by starting all trajectories aimed at a point 5.38 units from the origin. If there were no errors, the focus of the

beam would be 5.38 units back from the exit plane. The actual focus varied from 5.26 to 5.80 with an average error of six percent. The average radial position at the exit plane is two percent greater than at the entrance plane.

Fig. 7. Equipotentials (a) and electron trajectories (b) in a perveance 1.54×10^{-6} beam in a drift tube at 10 kV.

The Pierce theory⁸ for such a beam assumes the outer edge of the beam is at the drift tube potential. The equipotentials in Fig. 7(a) show that the voltage at the edge of the beam is depressed three to four percent from the drift tube voltage. For beams with a perveance greater than 10^{-6} A (volt)^{-3/2}, the beam current through the drift tube will rapidly become less than that given by the formula.

APPENDIX A

SNEER Input Data Description

The first four cards of the data deck largely control the flow and scaling within the program. The first card consists of 15 integers.

1. MM - The number of major cycles through the program; 1 for a space-charge free solution; larger, up to 10, for space-charge solutions.
2. KM - The number of cycles through the voltage matrix relaxation; up to 200 for a large matrix.
3. NBM - The number of "errors" in the beam border at convergence; generally 2.
4. NVM - The number of "errors" in the voltage matrix relaxation at convergence; generally 2.
5. NZ - The axial length of the matrix employed.
6. NR - The radial extent of the matrix employed.
7. NRO - The offset from the axis of symmetry to the bottom edge of the matrix; 9999 for rectangular configurations
8. MU - Controls the flow -
 1. First general solution.
 2. Second solution with different injected beam.
 3. Second solution with different electrode configuration.

The parameter MU extensively controls the flow of the program after the initial solution (MU = 1). If several solutions with differing initial beam conditions are desired (MU = 2) only the portion of the data involved

in setting up the initial beam needed by read for succeeding solutions. Several solutions with modified electrodes may be run with $MU = 3$.

9. NMR - Number of matrices used to describe the configuration to be simulated.
10. ISV - Not currently in use.
11. IST - Not currently in use.
12. IPLOT - Controls plotting; 0 gives no plot, 1 produces final trajectory plot.
13. IPR - Plot radius; if the trajectories are near the lower edge of the matrix, they may be obtained on a larger scale by specifying IPR as some value less than NR, $IPR = NR/2$ would double the size of the plot.
14. IPD - The print delete; 0 produces normal printing of voltage (and space-charge in SNEERA) matrices, 1 deletes this print.
15. KDI - The number of the JX matrix describing a dielectric surface where trajectories will or may be intercepted.
16. MPLT - Fore-shortens all plots produced by the factor $1/MPLT$. 1 or zero produces no distortion.

The second card consists of up to 14 integers (one for each integer matrix used to describe the electrodes to be described). Each number specifies potentials to be set on electrodes, and refers to the number of cards employed below.

The third card furnishes most of the scaling for the analysis

1. ZZERO - The Z position of the emission surface in scaled units.
2. VSCALE - The potential in volts to which all values employed on the voltage matrix are normalized.
3. ZSCALE - The length in meters corresponding to one scale unit.
4. DZ - The length of one matrix square in scaled units, e.g., if ten squares correspond to one scaled unit, $DZ = 0.1$.
5. EPSV - The maximum change at each point of the voltage matrix at convergence typically 3×10^{-4} (.03%).
6. PP - The ratio of the charged particle mass to its charge, normalized to that of an electron.

7. BETA - Over-relaxation constant for the voltage relaxation, typically 1.8.
8. EO - The initial energy (in volts) of the charged particles.

On the fourth card are:

1. BMAG - The normalization value in Teslas for the magnetic field to be read in below.
2. BRHO - The under-relaxation factor for the space-charge densities should be 1.0 or less.

The title card is then read. Anything punched on this card will be printed on the first page of the program output.

The next group of data describes any dielectric interfaces that may be employed. These cards are read if MU = 1 or 3. The first number on the first card is IEP and should be 0 if no dielectrics are employed and should be 1 if dielectrics are present. If IEP is zero, the remainder of the card may be blank and the next two groups of data describing interfaces may be omitted. If IEP is one, IDI (the second number) gives the number of vertical dielectric interfaces to be employed, and the rest of the card consists of the relative dielectric constants for consecutive pairs of matrices stored in the EP array.

The relative dielectric constants (EPV) across the vertical interfaces are then listed. The first two values are to the left and right of the first interface. The second and third values are to the left and right of the second interface. The third and fourth values are to the left and right of the third interface, etc. Note that there will be one more constant listed than there are actual interfaces. It may also be necessary to have "dummy" interfaces (see below) to make the dielectric constants come out right.

The interfaces are specified in detail on the ID matrix, each interface being described by a sequence of four numbers. The first number in

the sequence specifies the type of boundary at the lower and upper ends of the column. The possible boundary conditions are shown in Fig. 8. The six numbered lines at the bottom and tip of the interface are the only possible directions a dielectric boundary can take. Numbers (from 0 to 6) are used to tell the program the type of boundary to compute. The boundary conditions are given by a 4-digit number, the first two digits specify conditions at the lower limit and the last two digits specify conditions at the upper limit. A metallic boundary is given by the value zero, and the six possible dielectric configurations are shown in Fig. 8. Examples will be given in the sample plot discussion.

Fig. 8. Types of Possible boundary conditions at the top and bottom of a vertical dielectric interface; a, metallic boundaries; b, dielectric boundaries.

The next three numbers give the location of the interface. The first of these numbers is the column I, and the last two are the lower and upper J coordinates, respectively.

This sequence of four numbers is repeated for all such interfaces. If all four numbers are zero, the interface will be skipped, as would be the case when the dielectric constant list is not right for a particular interface.

The next group of cards specify the beam initial distribution. These cards are read for MU = 1 or 2. the first card in this group specifies first the number of cards to be used, ICS, and second the current (in amperes) in the beam, CRNT. Each card in the simulation contains a description of a portion of the distribution of current and trajectories:

1. JL - The lower limit of the emission region.
2. SL - The relative current density at JL.
3. AL - The angle the trajectory makes with the axis at JL in degrees.
4. BL - The relative magnetic flux density the trajectory has crossed between its emission point and its injection point into this program.
5. JH - The upper limit of this emission region.
6. SH - The relative current density at JH.
7. AH - The trajectory angle with respect to the axis at JH.
8. BH - The relative magnetic flux density crossed in arriving at the injection point JH.
9. CS - The spacing between trajectories in matrix square lengths, typically 1.0.
10. IT - The number of trajectories to be emitted from a point source: This should be zero for a distributed source. If IT is non-zero, JL must be equal to JH and the trajectories will be equally spaced between AL and AH. Only one point source is permitted. If more than one point source is desired, multiple runs can be made with MU = 2.

Relatively complex distributions of injection conditions can be simulated by overlaying several of these linear distributions. The only restrictions are that all the injected trajectories must be in one radial plane, and as

the program is shown in Appendix D, only 200 trajectories may be plotted. For the no-space-charge version of the program SL and SH are not employed at all.

The next card specifies an approximate beam border. Given are the coordinates of the two ends of a straight line. The initial beam border will be a straight line from IL, JL to IH, JH. Generally, this definition is not critical, but a good choice for a high space-charge density solution will speed convergence of the program. Matrices describing the electrodes are then read for MU = 1 or 3.

The electrode (and dielectric) configuration is specified by the integer matrices described above. Some restrictions and requirements will be listed here. As described above, dielectric interfaces sloping at 45 degrees or less to the axis or lower edge of the matrix are specified by making the upper limit matrix values, e.g., J(1,2), the same as the next lower limit matrix, i.g., J(1,3). Steeper interfaces must employ the radial interface technique described above. Also any electrode sloping at 45 degrees or less to the axis must be at least one matrix square thick.

The normal procedure in relaxing the potential is to compute the matrix starting at J(1,1), proceeding up the column to J(1,2), then from J(1,3) to J(1,4), etc. If any of these pairs is zero, it will be skipped. The reason for skipping a pair would be to obtain the proper dielectric constants at a dielectric interface.

Potentials may be set for MU = 1 or 3. Initial potentials are set by the following methods on electrodes, boundary points, and some dielectric interfaces if present. The first group of cards set linear potential distributions on radial columns on the voltage matrix. The first card specifies the number of such linear distributions. On each succeeding card are given

I, the column number; JL, the lower J limit; JH, the upper J limit, VSL, the voltage at (I,JL); and VSH, the voltage at (I,JH).

The second group sets axial linear distributions. Again, the first card specifies the number of such distributions. Each succeeding card gives; IL, the lower I limit; IH, the upper I limit; J, the row number; VL, the voltage at (IL,J); and VH, the voltage at (IH,J).

The third group is identical in form to the first group above, but sets logarithmic, radial, potential distributions. These distributions assume the same axis of symmetry as specified for the voltage matrix.

The fourth group permits the setting of potentials at individual points. The first card specifies the number of points, and each succeeding card contains I, J, and V(I,J).

The normalized values on the axis for the magnetic field are read in at this point if BMAG is non-zero.

The last potential setting section permits the setting of potentials along surfaces defined by the integer matrices defined above. Each card contains; IL, the lower I limit; IH, the upper I limit; and VSET the potential to be set along points defined by one of the JX matrices. The matrices to be used are specified on the second data card (see above) by values on the JJV matrix, JJV(1) corresponds to JX(1,1), JJV(2) corresponds to JX(1,2), etc. The number of potentials to be set is given for each matrix employed.

In all the above only non-zero values need be set, the matrix is initially all zero. Potentials within electrodes will be set automatically to the values set on the top and bottom surfaces. Non-zero potential electrodes on the axis (or bottom edge) of the matrix should be set to the proper potential on the bottom edge of the matrix. All of the above potentials should be normalized to VSCALE as defined on Card No. 3.

The next group of cards gives the information needed for plotting equipotentials and are read regardless of the value of MU. If an equipotential plot is desired, the potentials desired are listed on the next three cards. Up to 24 values may be plotted, if fewer are desired they must be listed consecutively. If the zero equipotential is desired, a value such as 0.0001 can be used.

If it is desired to expand any square areas of the plot, it is necessary to specify these areas on up to 5 cards giving the left and right, bottom and top coordinates on consecutive cards.

The data set is terminated with one blank card. The program may be terminated by 4 additional blank cards, or any number of additional data sets may be added. The last data set must be terminated with a total of 5 blank cards.

APPENDIX B

SNEER Data Sheets

The program SNEER actually exists in two forms--one with space-charge (SNEERA) and one with all space-charge and induced magnetic effects deleted (SNEERB). With the exception of the cards describing the initial beam conditions, the input data decks are identical.

SNEERA (B) DATA SHEETS

[illegible]

JX(3)

2013

JX(4)

2013

JX(5)

2013

2013

2013

2013

LL	RADIAL LINEAR				IT
I	L	N	V(I,L)	V(I,N)	8I4, 2E9
LL	AXIAL LINEAR				I4
L	N	J	V(L,J)	V(N,J)	3I4, 2E9
LL	RADIAL LOGRITHMIC				I4
I	L	N	V(i,L)	V(I,N)	3I4, 2E9
LL	POINT SETTING				I4
I	J	V(I,J)	2I4,EE9		

BM
 8E9

IL IH VS

214, E9

 VCON
 8E9

IL IH JL JH

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APPENDIX C

Sample Input Data

Sample input data for SNEER(B) are shown in Table 2. This is a tube which was found to be a suitable configuration for use as an ion gage to measure its own pressure. The trajectories are trapped by the magnetic field (0.02 tesla) and the decelerating electric field at each end of the tube.

Fig. 9. Trajectories and equipotentials for a trapped particle simulation.

of the trajectories are shown on the left. The envelope of the trajectories is actually nearly symmetric. The trajectories shown in Fig. 9 are overlaid on the equipotential plot.

The printed output for this run is shown in Table 3. Here maximum use has been made of the delete printing options to reduce the output to slightly more than one page. This run took 101 seconds on the CDC 6500. The angle and focus are printed for each trajectory, the angle being the angle between the Z-axis and the slope of the trajectory and the "focus" the point where the trajectory would cross the axis if extended forward (+) or backward (-) from the exist plane. In this case, these data are meaningless. The upper edge of the beam envelope is printed and shows that it is nearly symmetrical about the center of the plot. The number of time increments computed for each trajectory is also printed, the product of DT and the number of increments is the transit time.

APPENDIX D

SNEERA Compilation and Execution

The complete program consists of a main program called SNEER which performs most of the computations, several functions, and subroutines for saving and restoring data and plotting the output.

Subroutine TRPLOT handles the plotting of trajectories, and EQPLOT (along with CDPLOT, SCAN, TRACE, and CALC) handles the equipotential plots. These employ the North American Aviation Subroutines for the Stromberg-Carlson 4020 digital recorder, as modified for use on the CDC 6600 and 7600 computers at Sandia Laboratories, Albuquerque.

RDTAPE and WTTAPE restore and save data for possible restarts of a given data set. These employ the tape IST which is specified in the input data and would have to be listed on the program card if it were to be employed.

The execution is for the same input data as shown in Appendix C but with maximum printing by the program.

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