INSTITUTE FOR NUCLEAR SCIENCES VINČA
Physics Laboratory (010)

VERSION: **2KG**
January 2001

Radovan D. Ilić

SRNA-2KG

PROTONS TRANSPORT SIMULATION BY MONTE CARLO TEHNIQUES

(User's guide)

Beograd, Vinča, January 2001.

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1. PRESENTATION OF THE PROGRAMS FROM THE SRNA PACKAGE

SRNA software package is developed for simulation of proton transport by Monte Carlo method for numerical experiments in radiotherapy and dosimetry. Programs from this package run in 3D geometry, with arbitrary spectrum of proton from the source and with geometry of material zones that can be described by planes and second order surfaces. Actual version called **SRNA-2KG** runs in proton energy range from **100 keV to 250 MeV.** SRNA program uses probabilities of proton transition from previous to next stage of phased space that is prepared by the SRNADAT program.

The protons transport is based on a theory of condensed history [1] and on our model for compound nuclei decay that creates by protons absorption. On each part of range, an average loss of energy [2] is calculated with a fluctualation from Vavilov's [3] distribution with Schulek's [4] correction. Deflection angle of protons is sampled from Moliere's distribution [5]. Energy loss and protons deflection angle give data for the correction of proton range along axis (x,y,z) in cartesian coordinate system.

Compound nucleus decays with emission of protons, deuterons, tritons, alpha particles or photons. Their number is sampled from Poisson's distribution with appropriate average values of multiplication factor of each particle. Energy and angle of particle emission, and factors of multiplication are obtained from cross sections obtained by the integration of differential cross section [6] for nonelastic nuclear interaction. Energy and angle of secondary neutron emission are sampled from emission spectrums. Emitted photon will get an average energy. Transport of secondary protons is treated in the same way as proton transport from the source Neutron and photon do not treated. Emitted deuterons, tritons and alpha particles are absorbed at the place of their creation.

Software package SRNA is treating proton transport in materials which include elements from Z=1 to Z=92. Available cross sections for nonelastic nuclear interactions [6] for modest number of elements, limitate program application in numerical experiments. Programs from this package are written in FORTRAN 77, and run in double precision on common PC's which have MS Fortran PowerStation compiler. They can be used on other computers as well if routines for the clock and date change.

2. TRANSITION PROBABILITIE PREPARATION

Program SRNADAT prepares transition probabilities by successive run of its routines according to input data in double precision. Each routine performs numerical integration in order to create inverse distribution or probabilities after accomplishing the run. Separate database for each process is easier to control and more suitable for implementing new models. These procedures are very delicate because of the properties of density functions and conditions for using the theory of proton scattering are very sensitive.All of output data are formated and named *.PEC. Integration of density function is performed by Gauss-Legendre adapted formulae - DMLIN from IMSL and DQAG from Netlib. For numerical inversions we used splines, compatibile with time consuming. Distributions are inverted with preset probabilities in corresponding range to exclude interpolation in SRNA code, when that is possible. This model is easier for sampling numerous values in Monte Carlo simulation

2.1. Input data for SRNADAT

The latest necessary of data is input in file SRNADAT.INP. Routines of the code compute numerous constants and data needed for other routines by appling these data. SRNADAT.INP includes the following data:

MATA - Number of materials in the medium where passage of particles is simulated. All materials should be in accordance with data for geometry code RFG.FOR in RFG.INP. We recomanded user to prepare RFG.INP first, and after that SRNADAT.INP.

JMAT - Material or element number in file ICRU49.MAT for (dE/dx). If actual material do not exist in ICRU49.MAT, program run with Ziegler's data for (dE/dx). In this case JMAT must be great then 200.

GUST - Material density g/cm^3.

KOZONE - Number of elements in each material, whether or not a mixture of a compound.

JES - Flag: JES=1 compound; JES=0 mixture.

MZP - Ordinal number of the element in the Periodic system

NEZ - Number of elements in compound or mixture (for example: Al_2O_3 NEZ(1)=2 and NEZ(2)=3); or air: NEZ(1)=1, NEZ(2)=1 ….

UDEOT - Weight fraction (g/g) of element in material..

JON - Ion number; default value is JON=1 for proton.

EPOC - Minimal energy (MeV) in the energy scale.

EKON - Maximal energy (MeV) in the energy scale.

MFAK - Factor for creating energy scale from EPOC to EPEK. The MFAK is upgreating in the routine PREPAR according to the value DUNE.

KSUL - Flag for Sulek's correction in Vavilov's distribution. If KSUL=1 this correction is included. If KSUL=0 no Sulek's correction.

EPEK - Energy limit of type of energy scale. From EPOC to EPEK logarithmic scale, and from EPEK to EKON linear scale.

DUNE - Nominal energy loss factor according to the Vavilov's theory. Recommended value should be less then 0.05.

ECAT - Whitout these values for user is very important the minimal valeu of ECAT. That is a lower energy boundary (MeV) of proton where simulation is stooped and where its energy is absorbed at the point where the proton achieved the mentioned energy. ECAT is calculated in routine PREPAR. In SRNA.INP this energy can be greater then calculated ECAT.

Example*:* SRNADAT.INP for aluminum and water

```
  2                    MATA
116                    JMAT(1)
  2.698                GUST(1)
  1, 1                 KOZONE(1), JES(1)
  13                   MZP(1)
 1                     NEZ(1)
  1.000                UDEOT(1)
 180                   MAT(2)
  1.000                GUST(2)
  2 , 1                KOZONE(2), JES(2)
  1, 8                 MZP(2), MZP(3)
 2, 1                  NEZ(2), NEZ(3)
  0.1111, 0.8889       UDEOT(2), UDEOT(3)
  1,  1                JON, KSUL
  0.1, 100.0, 10.0, 0.05  EPOC, EKON, EPEK, DUNE
```

Program SRNADAT forms file SRDAT.OUT contained data from SRNADAT.INP and data resulting execution of the SRNADAT. File SRDAT.OUT should be saved in order to form input data file SRNA.INP. The data input in SRNADAT.INP must be in accordance with the parameter data in the SRDCOM.FOR. In this sence, the following values are important:

MTAC - Maximal expected number of points in the energy scale EST. Default value is 1601..
INMAT -Maximal number of different materials.
NELEM - Maximal number of elements for all materials. Default value is NELEM = INMAT*5...

2.2. Transition probabilities

The Routine of program SRNADAT prepare transition probabilities or needed numerical data. These routines are described here to show creation of transition probabilities.

ESKALA - Routine forms energy scale for protons. From EKON to EPEK scale is linear and from EPEK to EPOC scale is logarithmic. In this routine the scale factor MFAK prepared according to the value of DUNE. When routine PREPAR is finished, routine ESKALA forms file ENER.PEC.

DOMTABL - Routine calculate short pathlent of proton by numerical integration of 1/(dE/dx) from DEDX.INP (ICRU49 [2]) in the range EST(K) to EST(K+!), and data write in the file DERAN.PEC.

DOMZIEG- For materials or element hoes do not existing in ICRU49, this routine calculates short pathlent of proton by numerical integration of 1/(dE/dx) from Ziegler's model from TRIM, and results write in the file DERAN.PEC

MOLINV - Routine computes inverse Moliere's angular distributions by numerical integration of our prepared 5 Moliere's functions (MOLFUN.DAT) in the range from 0 to 40, using the routine DGAG from Netlib library. The inverse distributions as Cosine of deflection angle routine write in the file COSPAR.PEC.

AKSIVA - Calculation of the x in the Vavilov's distribution.

VAVIL - Routine computes inverse Vavilov's distributions by numerical integration with our model [3] using the routine DQAG from Netlib library, and the results write in the VAVINV.PEC.

SULEK - Using data for number of electrons and exitational potentials (SULEK.INP) for actual element, this routine computes Sulek's corrections of Vavilov's distribution. File EDER.DAT contains this data for each material as function of energy EST.

NONELN - Using cross section for nonelastic nuclear interactions ZXGEN.INP (Chadwick data form LANL) this routine computes integral of cross section along pathlent of proton The file NONEL.PEC contain data for average number of nonelastic events.

SEKPAR - Using differential cross section from Chadwick data file this routine calculates production probabilities for all actual particles.

NEMIS - Routine computes inverse emission spectra for neutron.

PEMIS - Routine computes inverse emission spectra for proton.

AEMIS - Routine computes inverse emission spectra for apha particles.

DEMIS - Routine computes inverse emission spectra for deuteron..

3. PROGRAM SRNADAT RUN

SRNADAT program is ready to start with input data in SRNADAT.INP file, which are in accordance with the filed dimension in SRDCOM.FOR and RFG.INP file. The file RFG.INP does not influence its run, but it is important to prepare it before the program SRNADAT run in order to enable the run SRNA program without problems.

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Preparation of the SRNADAT to run on common PC is simply a standard compilation and linking procedure. When this is finished, the program is started by SRDAT.BAT. During the run of program typical messages is shown on the screen, followed by messages of actual routine runs. It is foreseen the number of events in the loop for the routines with a longer run, especially the routine VAVIN.

Program SRNADAT forms separate SRDAT.OUT file with data witch should be completed with new data needed for the SRNA code. The user is advised to do this in accordance with the part of this manual describing SRNA.INP data file. After finishing execution of the SRNADAT we recommend user to see informational files MOLINF.PEC and VAVINF.PEC.

4. PROGRAM SRNA

Program SRNA.FOR is organized as main program, module, sections, functions and supported routine**.** Most of these units communicate using labeled COMMON without the list of arguments. All of values having the same meanings have unique names in all part of the SRNA code. A file called SRNACOM.FOR in which maximum dimension of arrays achieves this and constants are defined by the PARAMETER statement and by labeled COMMON. The file SRNACOM.FOR is included in SRNA.FOR during compilation.

4.1. Input data for SRNA

Two groups of input data are used by SRNA code. The first group is data contain spectrum and geometry of the proton source, and data describing material zones and computational conditions. The second group includes probabilities prepared by the SRNADAT code. The third group is created by the PARIP routine from mentioned two groups. Numerical experiment by SRNA code need user's input data from file SRNA.INP. This input data obtained by adding new input data to the previously created file SRDAT.OUT data file. New data are added according to the established order and have the following meaning.

LUZON - Number of geometry zones in accordance with geometry input data RFG.INP file, including vacuum between zones.

JGEOM - Geometry type flag:
JGEOM=101 - 1D slabs orthogonal to the Z-axis;
JGEOM=202 - 3D geometry's with circular cross section of proton beam with axis in 4π;
JGEOM=303 - 3D geometry's with rectangular cross section of proton beam with axis in 4π.
JGEOM=404 - 1D geometry's with rectangular cross section of proton beam with axis in 4π.

AKV, BKV - Half of the bases of rectangular beam cross section for JGEOM=303 and 404.
NZ - Ordering numbers of the zones Znn in RFG.INP.

MATZ - Vector having LUZON values. Each material region has its corresponding number with the order of data prepared by SRNADAT.FOR. Vector MATZ enables the geometry regions to be 'filled' with one material or a combination of materials within given geometry. For example MATZ(1) = 1 and MATZ(2) = 2, means that the second material is behind the first one. If MATZ(1) = 2 and MATZ(2) = 2, means that the first material is behind the second one. The user might already see the possibilities of assigning the values to the vector MATZ when the number of material regions is bigger, at least 5. So, for example if one would like to study the influence of a few materials or their order on the simulation process it is enough to input the wanted values in the vector MATZ. Application of the values MATZ(N) = -1 is especially important if one of the regions is considered as vacuum. SRNA code excludes that region and the particle crosses the border of the next zone.
DEBLJ - Vector with data of optical lents along Z-axis for calculation of absorbed energy as a function of target depth only if JGEOM=101.and 404. In this case absorbed energy is showed in MeVcm^2/g. in SPSRNA.DAT file.
KORAK - Vector with a number of steps which will divided lents DEBLJ only if JGEOM=101.
XTM, YTM, ZTM - Coordinates of target center.
RSN - Beam radius; for pencil beam RSN=0.
RSF - Biggest sphere radius with center in point (0,0,0) around of target. This radius must greater then 10 time the radius RSN.
TETS - Polar angle of proton beam in degree.
FITS - Azimuthal angle of proton beam in degree.
NSLIN - Number of lines in differential energy spectrum of the proton from the source. It is assumed that the source is given in the form of histogram. Routine PARIP prepare inverse energy distribution. Normalized spectrum is not necessary because the routine PARIP performs normalization.
NPOC - Total number of particles from the source should be 20k, where k = 1, 2, 3, … , in order to run the code with 20 batches, enabling statistical regularity of the simulation error.
TIMCAT - Preset time (minutes) after which program is terminated.
ENER - Vector with NSLIN values of energy spectrum of the particles from the source. Inverse distribution from the PARIP routine is input in this vector.
UDEOE - Fraction of the line in the energy spectrum of the particle from the source.
DEBX, DEBY - Half of the bases of parallelepiped in plane XOY for subdivision of the space on elements.
DEBZ - Height of parallelepiped along Z-axis.
ISLIK, JSLIK, KSLIK - Number of steps for the space subdivision along coordinate axis, and for the absorbed energy (MeV/kg) distribution image from the file SLIKA.DAT by GRAF.FOR. For energy fluens ETRANS.DAT program used KSLIK steps.
TEMAX- Maximal polar angle for angular distribution leaking protons along Z-axis in ANGULAR.DAT file.
JTEF - Number of channels for ANGULAR.DAT.

Previously described input are added to SRDAT.OUT file renamed as SRNA.INP, as follows:

LUZON, JGEOM
NZ, MATZ(I), **DEBLJ(I), KORAK(I)**
XTM, YTM, ZTM
RSN, TETS, FITS, RSF
AKV, BKV
NSLIN, NPOC, TIMCAT
ENER(K), UDEOE(K)
DEBX, DEBY, DEBZ
ISLIK, JSLIK, KSLIK
TEMAX, JTEF.

RFG.INP - input file read and used by geometry module RFG. It contains data describing geometry of the material region where particles transport occurs. Data are input in the manner typical for RFG. The following example illustrates an aluminum and water slabs in sphere.

```
C   [ Sphere + 3 planes ]
C   [ Sphere: x^2 + y^2 + (z)^2 = 50^2 ]
C   [ 1 Plane : z=0.0 ]
C   [ 2 Plane : z=0.0180 ]
C   [ 3 Plane : z=10.018 ]
D1  [ OBLIK=3; JED=2; KOEF = 50.0, 50.0, 50.0 ]
D2  [ OBLIK=2; JED=1; KOEF = 0.0, 0.0, 1.0, 0.0 ]
D3  [ OBLIK=2; JED=1; KOEF = 0.0, 0.0, 1.0, 0.0180 ]
D4  [ OBLIK=2; JED=1; KOEF = 0.0, 0.0, 1.0, 10.018 ]
C   [ Complex space ]
D11 [ OBLIK=1; LOGIC= 1 I 2 ]
D22 [ OBLIK=1; LOGIC= 1 I 3 ]
D33 [ OBLIK=1; LOGIC= 1 I 4 ]
D12 [ OBLIK=1; LOGIC= 22 I -11 ]
D13 [ OBLIK=1; LOGIC= 33 I -22 ]
D14 [ OBLIK=1; LOGIC=  1 I -33 ]
C   [ Material zones  ]
Z1  [ DOMEN = 11 ; MAT =-1 ]
Z2  [ DOMEN = 12 ; MAT = 1 ]
Z3  [ DOMEN = 13 ; MAT = 2 ]
Z4  [ DOMEN = 14; MAT =-1 ]
Z5  [ DOMEN =-1  ; MAT =-2 ]
K   [ End of data ]
```

4.2. Preparation SRNA code for execution

It was mentioned in the introduction that SRNA code has very wide application possibilities. It enables the user to choose the geometry of the material regions and the source without any constraint, as well as the properties of the source and the options to treat the parameters resulting from particles transport. Certainly, it is expected from the user to understand these options and include relevant changes in the original code.

First of all, dimensions of vectors in PARAMETER statements should be defined in the SRNACOM.FOR file. The following parameters for adjustment are available to the users:

IGMAN - Maximum number of geometry regions in the SRNA.INP file. All the distributions dependent on the material have at least one dimension IGMAN. That is why IGMAN should be carefully chosen first.
LNE - Maximum number of lines in the energy table EST for proton; LNE greater or equal to MTAC is recommended.
LEL - Maximum total number of the elements in all the material regions. This number has the same meaning as NELEM in SRDCOM.FOR.

KCLT - Number of packages into which particles from the NPOC source are divided. It enables application of the central boundary theorem for estimating the statistical error for the sum of random values which obey Gauss distribution. For statistical regularity number of packages should be at least 20 as it is already preset in the SRNACOM file.

LIZV - Maximum number of lines in the energy spectrum of the source particles. Number greater than NSLIN is desirable.

Once when all the needed values are input in the SRNACOM.FOR file, depending of nonstandard geometry case, it is necessary to adapt the routines marked POCTAC* for the defined protons source.

Preparing the SRNA code for execution means standard compilation and link procedures, or using SRNALIN.BAT to obtain SRNA.EXE, and starting with SRNA.BAT.

4.3. Execution of the SRNA code

SRNA code starts execution by reading all the data created by SRNADAT, input data SRNA.INP and RFG.INP. After testing the input data and possible interruption for sending messages in a case some error occurred, control module TRANSP starts execution calling sections for simulation. From the beginning of the SRNA code run a typical message is written on the screen, followed by the data read. A text informing the user about the type of interaction performed and about the conditions of simulation follows. Next comes the text describing which of the 20 packages is treated with the number of particles included in the computing, time elapsed and the time left for terminating the code run.

4.4. Choice of random values of the distribution

Numerical simulation of particles transport by Monte Carlo techniques demands a large number of choices of random value series from their distributions. Acceptable statistical error demands simulation of transport of a great number of particles. These are the reasons for simple and quick choice of random values. Since common geometry module is quite time consuming it is even more important to simplify and accelerate the choice of random values.

SRNA code applies our models for choosing random values from their inverse distributions. Inverse distributions are written index wise as solution for the chosen distribution per variable. Model of probability constant increment from zero to one is applied for calculating of inverse distributions. Number of increments is chosen according to properties and flow of the distribution. Some distributions are inverted with logarithmic increment of probability in the range from P_{min} to one. Index and value of the random variable for inverse distributions with constant probability increment are chosen by choosing random number RJ = DRAN(ISEED). Index of the random value is easily obtained as M = 1 + NNN*RJ. Random variable is then easily used from the XS(M) vector. Choice of the random variable from inverse distribution formed by logarithmic increment is performed by M = 1 + NDN*ALOG10(En/Ep)/ALEM, while the random variable is obtained from YS (M). Besides choosing random variables in the SRNA code a necessity exists for search of the cross section closest to the value in the cross section library for the particle energy needed. Organization of this search is similar to that of the random variable, the only difference being that the needed energy is not a random value.

4.5. SRNA output files

After ending of the SRNA code execution, i.e. after ending numerical experiment, the following output file is available:

SRNA.REZ - contains material data with elements of its constituents, informational data about conditions for probabilities preparation, some simulation conditions, and absorbed energy per zone with statistical errors and CPU time and date as ‘Day Mount Year’.

SLIKA.DAT - contains data for absorbed energy in elements of space in MeV/kg. Program GRAF.FOR extracts data for graphical presentation of energy distribution.

SPSRNA.DAT - contains data of absorbed energy along Z-axis in (MeVcm2/g) only if .

ANGULAR.DAT - is an angular spectra from target of leakage protons along Z-axis.

SPECTRUM.DAT - is an energy spectra from target leakage proton along Z-axis.

ETRANS.DAT - is an energy fluens of protons through target.

SURC.DAT - Space distribution of place where incident proton generated neutron or photon.

5. GEOMETRY MODULE RFG

RFG.FOR code belongs to the code family for describing the geometry of material regions and calculating geometry parameters of the particle that moves linearly between two collisions. RFG.FOR is applied in SRNA code as a geometry module to calculate the distance between the point of particle position and the boundary of the nearest geometry region DDD (KZ=1), and to determine the index of the particle geometry IDD (KZ=1). After input of all the data SRNA code calls routines RFG.INP, RFGPRE, RFGPRE1 and RFGPRE2 which read RFG.INP and its library RFG.DAT belonging to RFG.FOR. Thus conditions are fulfilled for running the RFG module. Sections PARTRAN call the routine NEAREST which gives the logic variable INTERS. If INTERS=.TRUE., NEAREST has determined the demanded data: DDD (KZ) and IDD (KZ). On the contrary there is no contact with the geometry regions - the particle is outside the material region.

SRNA code communicates with the module RFG.FOR by means of COMMON/INTS/. Coordinates (RX, RY, RZ) of the point position and the vector of its velocity (AX, AY, AZ) are important for its execution. Values of the nearest distance EL = DDD (KZ) are given in the same units as coordinates (RX, RY, RZ)..

5.1. Input data for RFG.FOR

Input data for RFG.FOR code are written in the RFG.INP file according to the model established by its author Dr Dimitar Antiparmakov. Besides the recommendation to the user to look up the source literature concerning RFG codes, a short description is given here needed for preparing the RFG.INP input file. All the variables in RFG.INP file are in open format. Each record of 80 characters has the following form:

MI (i) [P1 = U11, U12, ..., P2=U21, U22, ..., P3=U32 ...] TEST

Identifier MI has the following values:
C - comment
D - definition of geometry parameters
Z - definition of material region
K - end of data
i - index of the record; i=1,2,3,...,99 for records of D and Z type.

Parameters P1, P2, … in records D are: P1 = OBLIK = 1 to 11 dependent on the type of equation in Table of Appendix.

P2 = **JEDN** = 2 standard type of equation in Table of Appendix,
P3 = **KOEF** = parameter **A, B, C, D** or **a, b, c** in Table,
P4 = **LOGIC** = **I** for intersection, **U** for union
P5 = **TRANSL** = X0, Y0, Z0 in equations

Parameters in Z records are:
DOMEN = definition of geometry region
MAT - index of material region that is not used in RFG.FOR, but it is recommended to input all the MAT values for easier control of data in SRNA.INP.

Preparing the data for writing records in RFG.INP demands the user to find the simplest geometry forms for parts of space inside the given geometry regions which would present the geometry in RFG logic in the simplest manner. Examples of few configurations are given in the Appendix.

5.2. Control of data in RFG.INP

Contents of RFG.INP file, correctly input according to the instructions in this section, would describe geometry and material regions. Very often this is not the case. Misunderstandings arise because dimensions of material regions (geometry bodies) are taken from design drawing and not from a drawing in coordinate system. Another mistake happens because dimensions must be summed along the coordinate axes. Code RFGT should be applied for control of data in RFG.INP file which gives results of check-up according to the users demands. That code is located in folder RFGTEST. Lot of the examples for RFG.INP located in folder RFGLIB.

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APPENDIX

Table. Indications of standard RFG equations

Shape	Region	Standard equation
1	**Complex**	**Logic formule**
2	**Halfspace**	**$-Ax - By - Cz + D = 0$**
3	**Ellipsoid**	**$1 - (x/a)^2 - (y/b)^2 - (z/c)^2 = 0$**
4	**One-side hyperbloid**	**$1 - (x/a)^2 - (y/b)^2 + (z/c)^2 = 0$**
5	**Two-side hyperboloid**	**$1 - (x/a)^2 + (y/b)^2 + (z/c)^2 = 0$**
6	**Elliptic cylinder**	**$1 - (x/a)^2 - (y/b)^2 = 0$**
7	**Hyperbolic cylinder**	**$1 - (x/a)^2 + (y/b)^2 = 0$**
8	**Conus**	**$- (x/a)^2 - (y/b)^2 + (z/c)^2 = 0$**
9	**Elliptic paraboloid**	**$- (x/a)^2 - (y/b)^2 + 2z = 0$**
10	**Hyperbolic paraboloid**	**$- (x/a)^2 + (y/b)^2 + 2z = 0$**
11	**Parabolic cylinder**	**$- (x/a)^2 + 2y = 0$**

Note: For editing RFG.INP, please see examples on RFGTEST.

Obligations

Author of the SRNA code package guarantees that it operates correctly under the circumstances described in the manual. If the user would find some difficulties working according to the instructions the author is ready to help as soon as possible. The author is expecting the users to inform him about the problems which arise during application of the SRNA code package and results obtained by numerical simulation which would help improvements of the software. The author is obliged to inform all the users about the possible changes and improvements of the codes periodically.

Radovan D. Ilic, PhD
E-mail: rasacale@beotel.yu; URL: http://www.beotel.yu/~rasacale