9. *References:* R. A. Pfeiffer and W. W. Stone, TRAM for the Philco-2000. KAPL-M-RPC-1 (March 24, 1961).

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LOS ALAMOS LEAST SQUARES

1. Name of code: Los Alamos Least Squares
2. Computer for which code is designed: IBM 704
   Programming system: FORTRAN II
3. Nature of problem solved: Least squares fitting of linear or nonlinear functions in several independent variables. Thus, the program determines an estimate of A in the function $y = f(X; A)$ by means of minimizing the sum of squares. In the function, X is a vector of observed variables and A is a vector of parameters to be determined. In this context, a linear function is one whose partial derivatives with respect to the elements of A are all independent of A; a nonlinear function has at least one of the elements of A appearing in at least one of these partial derivatives. An example of a linear function is the usual linear regression model $y = XA = a_1x_1 + a_2x_2 + \cdots + a_kx_k$. A nonlinear function is the sum of exponentials model $y = a_1e^{a_2x} + a_3e^{a_4x} + \cdots + a_{k-1}e^{a_kx}$.
4. Method of solution: The iterative method of Gauss (sometimes called the Gauss-Seidel method) is used. The function is expanded with respect to A in a first-order Taylor's series about some point A_0. A vector of "corrections," say D, is obtained by multiple regression methods and a new estimate $A_1 = A_0 + D$ is obtained. The process is repeated until the vector D is "sufficiently small." The function and its derivatives with respect to the parameters are supplied to the program by the user by means of a subroutine.
5. Restrictions on complexity of problem: As originally conceived, the program was written for a 32K memory and would handle up to 500 data points, up to 5 independent variables, and up to 20 parameters. Different versions of the code are written for various memory sizes; 8K is usually sufficient, but it can be scaled to 4K. No restrictions have so far been encountered as to the nature or complexity of the function as long as no discontinuities exist in the function or its derivatives over the range of usefulness; i.e., the data must be physically significant, "well-behaved," and reasonably describe the function to be fitted. The Los Alamos 704 underflow is automatically set to zero, and the code does not check UV-OV conditions. Program and data are read on-line, with output going to BCD Tape 9.
6. Running time: Varies widely depending upon number of data points, parameters and independent variables; from 5 sec to 5 min. From 5 to 15 iterations are usually sufficient.
7. Unusual features: A damping factor is introduced to help control nonconvergent oscillations. Estimates of the standard deviation of all parameters are included with the solutions. Any (or all) parameters may be held at constant values. Arbitrary weighting of the observations y is permitted. The program package is "subroutine-ized" so that its various parts are easily modified or incorporated into other programs.
8. Present status: Several programs developed during the evolution of the present general code are currently operating at various Laboratories under such names as FRENIC, PEERLESS, and EXPO. 7090 Monitor versions are now being developed.
9. *Reference:* R. H. Moore and R. K. Ziegler, The solution of the general least squares problem with special reference to high-speed computers. Los Alamos Scientific Laboratory Report LA-2367 (October 15, 1959). This report contains a more complete set of references.

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9-RENUPAK (UNC-90-1)

1. Code designation: 9-RENUPAK (UNC-90-1)
2. Computer and programming system: Program is written in [F.A.P.] for the IBM-7090. A 32K core and ten tape units are required.
3. Problem solved: 9-RENUPAK treats the penetration of an infinite, homogeneous medium by neutrons from a point or plane isotropic source. The energy spectrum of the source must be continuous so that, for example, strictly monoenergetic source problems are excluded. The code output gives the neutron flux and current for both point and plane isotropic sources, as well as an integral over energy of the flux times an arbitrary response function, i.e., dose, activation, etc.
4. Method of solution: Computation is based on the moments method (*1–5*). After the moments are computed they are used to reconstruct the flux and current. The flux is assumed to consist of a linear combination of functions of given form, and constants in the expansion are adjusted so that the moments of the linear combination are the same as the computed moments of the flux.
5. Physics approximations: In the elastic slowing down treatment the neutron energy-angle relationship is taken into account properly. The code treats both elastic and inelastic scattering of neutrons. The inelastic scattering of neutrons is assumed to be isotropic in the laboratory system with a choice of several nuclear models in computing its energy dependence. In particular, the code allows for both discrete energy levels (when the levels are well separated) as well as a continuum of energy levels when the levels are very close. For heavy materials a statistical model is available.
6. Restrictions on complexity of problem: Maximum number of groups $\leqq 400$, isotopes $\leqq 5$, response functions $\leqq 16$. Only Gaussian and exponential fits available at present.
7. Typical running time: A typical calculation with 200 energy steps and 8 response functions, yielding both Gaussian and exponential fits for both point and plane source, takes about 12 min on the IBM-7090.

8. Status: Code is in use and available through United Nuclear Corp. Contact S. Preiser for additional information.
9. *References:*

1. J. CERTAINE, A solution of the neutron transport equation, Part II: NDA-Univac moment calculations. NYO-6268 (NDA 15C-53) (May 1955).
2. J. CERTAINE AND J. BROOKS, Addition of inelastic scattering to the Univac moments calculations. NDA 2015-92 (December 1956).
3. H. GOLDSTEIN, "Fundamental Aspects of Reactor Shielding." Addison-Wesley, Reading, Mass., 1959.
4. J. CERTAINE, A solution of the neutron transport equation, Part III: Reconstruction of a function from its moments. NYO-6270 (NDA 15C-61) (July 1956).
5. J. CERTAINE, E. DEDUFOUR, AND G. RABINOWITZ, RENUPAK, An IBM-704 program for neutron moment calculations. NDA 2120-3 (December 1959).

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9-NIOBE (UNC-90-2)

1. Code designation: 9-NIOBE (UNC-90-2)
2. Computer and programming system: Program is written in [F.A.P.] for the IBM-7090. A 32K core and ten tape units are required.
3. Nature of problem solved: 9-NIOBE solves the time independent multienergy neutron or gamma ray transport equation in a finite multilayered spherical configuration.
4. Method of solution: the computation can be broken down into two components, namely:
   (a) the slowing down treatment
   (b) the solution of the "one velocity" problem.

   In the elastic slowing down treatment, the neutron (or gamma ray) energy-angle relationship is taken into account properly. The code treats both elastic and inelastic scattering of neutrons. The inelastic scattering of neutrons is assumed to be isotropic in the laboratory system with a choice of several nuclear models in computing its energy dependence. In particular, the code allows for both discrete energy levels (when the levels are well separated) as well as a continuum of energy levels when the levels are very close. For heavy materials a statistical model is available.

   The treatment of the solution of the "one velocity" Boltzmann equation is based on solving the integral form of the equation iteratively. Assuming a value for the angular flux, the "one velocity" equation is solved by integrating along the characteristics arising from a classical treatment of the first order partial differential equation. The process continues until two successive iterates agree to within a specified tolerance. Lagrange interpolation up to order fifteen is used on the angular variable, while all integrations over the angular variable are accomplished by Gaussian quadrature. Finally, an overrelaxation technique is employed, and convergence to the angular flux in a physical problem is expected.

   The cross section data required consists of the total and scattering cross sections, the Legendre coefficients of the differential scattering cross section (up to order 19), and appropriate data for inelastic scattering. The data are tabulated against energy, and the set of values required are computed by the code from these basic tabulations. The radiation source may be specified either as incident on the configuration or may be internally distributed.
5. Restrictions on complexity of problem: At each of a maximum of 200 radial points, 9-NIOBE calculates the angular neutron (or gamma) flux in a maximum of 16 directions, at a maximum of 200 energy values (spaced equally in increments in $\ln E$ for neutrons; spaced equally in wavelength for photons). At present, a maximum of five materials is permitted in each region, and up to fifty regions may be handled.
6. Typical running time: A typical problem having 85 radial meshpoints, 81 energy values, and 8 angular rays required $2\frac{1}{2}$ hr on the IBM-7090.
7. Status: Code is in use and available through UNC. Contact S. Preiser for additional information.
8. *References:*

1. J. CERTAINE, A solution of the neutron transport equation—Part II. NDA-Univac Moment Calculations, NYO-6268 (1955).
2. J. CERTAINE, Integral term for elastic scattering of particles. NDA 15C-12 (1953).
3. J. CERTAINE AND J. BROOKS, Addition of inelastic scattering to the univac moment calculations. NDA-2015-92 (1956).
4. H. GOLDSTEIN, "Fundamental Aspects of Reactor Shielding," Addison-Wesley, Reading, Mass., 1959.
5. S. PREISER, G. RABINOWITZ, AND E. DEDUFOUR, A program for the numerical integration of the Boltzmann transport equation. NIOBE ARL Technical Report 60-314.
6. J. CERTAINE, E. DEDUFOUR, AND G. RABINOWITZ, RENUPAK, An IBM-704 program for the neutron moment calculations. NDA 2120-3
7. D. YETMAN, B. EISENMAN, AND G. RABINOWITZ, Description of input preparation and operating procedures for 9-NIOBE, an IBM-7090 code. NDA 2143-18 (1961).

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