

The SITHA Code

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Abstract

The SITHA (Simulation Transport HAdron) is a Monte-Carlo transport code. It allows simulation of protons, neutrons and charged pions transport through matter blocks of a complicated geometry. Simulation is performed for all hadrons with energies from 20 MeV to 10 GeV and it is performed only for neutrons with energies below 20 MeV. The main physical approaches of the SITHA code as well as its structure are briefly described. Some attention is devoted to our last investigation of the different systematics of double differential spectra of emitted nucleons from the inelastic hadron – nucleus interactions.

Introduction

The creation of the SITHA code started in the Khlopin Radium Institute in 1983 and the first version was developed in 1984^{/1/}. Since that time the code has been developed continually^{/2,3/}. The main purpose was to develop a code would allow us to get fast estimations of different types electronuclear reactors target characteristics. Simulation of the hadron transport has been the only way for reliable estimation of these characteristics because of insuperable difficulties of accurate analytical or approximate numerical methods arise when they are applied to calculation of complex geometry and high inhomogeneity constructions. At that time we have not any real possibilities to use the existing transport codes: NMTC^{/4/}, HETC^{/5/}, SHIELD^{/6/}, MARS^{/7/} and we known their principal difficulties. Moreover we were needed a code which might be easily modified by us.

During approximately ten years the SITHA code has been converted from a small program with limited aims into a large package of codes with different possible applications. It is interesting that the structure of the main part of the code has not seriously changed from the first version. It describes protons, neutrons and charged pions transport in the energy interval from 20 MeV to 10 GeV and it describes only transport of neutrons with energies below 20 MeV. In the second case the details of the thermalization effects may be taken into consideration for neutrons with energies less than 5 eV. This last capability of the code will not be discussed here more in detail. The different libraries of cross sections prepared by us^{/2,8/} are used in the SITHA code Fig.1. Additionally, part of ENDF/B-VI library ($MF = 7$) immediately used in the case of simulation of neutron thermalization is included in the calculation. The various kinds of results schematically presented in Fig.1 may be obtained with SITHA code. The first version of the code has been realized in a computer compatible with a IBM-360. Today the SITHA code has been installed on the following computers: VAX, ALPHA, SUN.

Theoretical and computational approaches

The SITHA code consist of the two main parts which are conventionally called the "FAST", describing the transport of particles with energies above than 20 MeV and the "SLOW" describing the transport of neutrons with energies below than 20 MeV. First we describe the main approaches used in the "FAST" part of the code. The "SLOW" part will be described latter.

There are two approaches to the hadron transport simulation – "exclusive" and "inclusive", which are being distinguished by means of representation of inelastic hadron-nucleus interaction. The first approach is based on a direct statistical simulation of processes for cascade, pre-equilibrium, and evaporation stages of the inelastic interaction. In contrast with the "exclusive" approach the "inclusive" one is based on solving the system of linear integral equations of hadron transport by using the method of Monte-Carlo simulation

$$\psi_i(x) = \sum_j \int A_{ij}(x, y) \cdot \psi_j(y) \cdot dy + \psi_i^0(x)$$

where ψ_i is the density of interactions of the hadrons of type i , $x \in (\vec{r}, \vec{\Omega}, E)$ is a point of the phase space, $A_{ij}(x, y)$ is the kernel function of the integral operator A_{ij} which may be presented as a convolution of the interaction operator K_{ij} with the transport operator T_{ij} . Here a description of the inelastic hadron-nucleus interaction is realized by means of simulation of double differential cross sections as a factor in the kernel function of the operator K_{ij} . Thus, an accurate description of intranuclear processes and a reliable representation of inclusive spectra are necessary for successful simulation of the inelastic interaction in the framework of the "exclusive" and "inclusive" approaches respectively.

The SITHA code is organized in a way allowing the application of two discussed approaches, but the main calculations have been made using the "inclusive" approach. The D2N2 and EVAP codes^{/9/} are used as a part of the kernel function of the interaction operator K_{ij} . It is difficult to simulate energies and directions of the particles emitted from the inelastic interactions using this codes immediately. By this reason the weight method is used. In each inelastic interactions we simulate emission of five particles. They are a proton, a neutron and two charged pions which are linked with a part of the kernel function $K_{ij}(x, y)$ describing the processes of quasi-elastic scattering, cascade and pre-equilibrium stages of

interaction. The fifth particle is a neutron which is linked with the evaporation stage of the interaction. In this case the simulation of neutron energy is based on the EVAP code which calculates the temperature of the neutron spectrum and the mean values of the evaporated neutrons. It is supposed that the angular distributions of the evaporated neutrons is isotropic in the laboratory system. In the first case the energy of the particle is selected uniformly on the logarithmic scale from the energy of the incident particle to E_{min} which has the value of 4 MeV in our code. The emission angle of the particle is simulated in the interval from 0 to 180 degrees with the following function

$$f(E, \theta) = \frac{A}{E} \cdot \exp\left(-\frac{E \cdot \theta}{\tau}\right)$$

where A is a normalization coefficient and

$$\tau = \frac{200 \cdot E_0}{500 + E_0}$$

here E_0 is a kinetic energy of the incident particle. The statistical weight of emitted particle is equal

$$W_i = \frac{d^2 N_i}{dE d\Omega} \cdot 2\pi \cdot \ln\left(\frac{E_0}{E_{min}}\right) \cdot f^{-1}(E, \theta)$$

The simulation of the elastic scattering is based on the classic optical diffraction theory valid for small angle scattering. The transport of the charged particles between two nuclear interactions is simulated with the assumption of the continuous ionization energy loss. The multiple Coulomb scattering is taken into consideration.

The total and inelastic cross sections of the hadron interactions with atomic nuclei in the energy interval from 20 MeV to 10 GeV are contained in the HECSF (High Energy Cross Section File). This library has been organized by us^{/8/} in the format similar to the ENDF-5 format. We saved the internal structure of the ENDF-5 format, but use own numbers of file (MF) for charged particles. It contain information about eight atomic nuclei (H, He, Be, Al, Fe, Cd, Pb, U). A double logarithmic interpolation is used for the atomic nuclei which are absent from the library

$$\sigma(A) = \sigma_1 \cdot (A_1/A_2)^x$$

$$x = \frac{\ln(\sigma_2/\sigma_1)}{\ln(A_2/A_1)}$$

where σ_1 and σ_2 are the cross sections of the two atomic nuclei from the HECSF with atomic weights A_1 and A_2 consequently. Part of the data from the HECSF is presented in Fig.2. For a comparison, the total neutron cross section for lead from the ENDF/HE library^{/10/} is showed by a dotted line. There is good agreement between our old data and the data of the contemporary estimation^{/10/}.

The simulation of the neutron transport with energies below 20 MeV is based on the multigroup neutron cross section library GR175-V1 developed by us^{/2/}. The 175 energy groups with 5 subgroups in the resonance region are used in our library. The simulation of neutron interaction with atomic nuclei is done in two stages. At the first stage the type of atomic nucleus is selected by using the macroscopic total neutron cross sections of all nuclei presented in the mixture. At the second stage the energies and directions of the emitted neutrons are simulated using individual characteristics of the selected nucleus. Our scheme of the multigroup neutron cross section preparation from the evaluated neutron data libraries is shown in Fig.3. It is realized only in computers comparable with IBM-370 and higher models working with the VM operation system. Because the main procedures controlling the connection between different codes have been written by REXX language. We use a part of well-known codes^{/11,12/}. The available elements are presented in Table 1.

One of the central parts of the Monte-Carlo transport codes is occupied by the geometry package. There are three various geometry packages used in the SITHA code. The difference between them involves the methods of geometry description and the fields of applications. The first package describe the geometry of objects using a number of standard surfaces. Each surface may be arbitrary placed in the space and may have arbitrary orientation relative to the main coordinate system. This

package is used mainly for the description of objects with a very complicated shape. The second package is based on using a number of volumes obtained one of the basic geometrical shapes. The volumes may be placed and oriented in the space arbitrary. Also one volume may be inserted into another. This package is mainly used for the description of the multidetector experimental setups. The third package is used for the simulation of the particles transport in the Earth atmosphere.

A scheme illustrating the structure of the main SITHA subroutines is presented in Fig.4. The names of subroutines to some extent describe their roles in the code.

Systematics of double-differential spectra of emitted nucleons

As it was discussed above the success of the "inclusive" approach used in the SITHA code depend on adequate representations of double differential spectra of secondary particles in the whole range of kinetic energies and angles of their emission induced by primary particle with kinetic energies from a few tens of MeV's to a few GeV's. A review of the main approximation systematics has been presented in^{/13/}.

One can note a large diversity in double differential spectra representations and in regions of their application. Some systematics^{/9,10,14-16/} have been compared^{/17/} with experimental data on inelastic scattering of protons by a thin Pb-target^{/18/} and between themselves for primary nucleons with kinetic energies from 50 MeV to 1000 MeV. Partially this comparison is presented in Fig.5 and in Table 2. It has led to conclusion about the necessity of further modification of the existing approximations or creation of new systematics.

To receive correct results in the framework of the "inclusive" approach double differential spectra systematics must fit not only a separate experimental result but they must be a self-consistency on energy conservation law. As shown in^{/13/} a confident description of an individual experiment does not eliminate an error of integral quantity derived from the data. Possible errors of measuring together with a lack of control of integral quantities derived from all nuclear reaction channels can lead to serious errors when the "inclusive" approach is used for simulation. Therefore systematics by Sychev e.a. (1979) is more reliable but it has no simple structure and that makes an impossible its future development.

Pearlstein's (1987) systematics as follows from our consideration^{/13/} is more attractive in view of modification convenience and possibility of spectra representation in the wide region of secondary particle energies and emission angles

$$f(E, \theta) = E \cdot \sum_{n=1}^N a_n(\theta) \cdot \exp\left(-\frac{E}{t_n(\theta)}\right),$$

$$a_n(\theta) = \sum_{i=0}^2 a_{n,i} \cdot P_i(\cos(\theta)), \quad t_n(\theta) = \sum_{i=0}^2 t_{n,i} \cdot P_i(\cos(\theta)),$$

where G is a function describing a peak of a quasi-free scattering. This systematics has been modified including the conservation laws for function minimization. To see the fit spectrum transformation two function have been minimized:

$$F_1 = \sum_{l=1}^L \left[\sum_{i=1}^{M_l} \frac{1}{W_{il}^2} \cdot \left(\ln \frac{f(E_{il}, \theta_l)}{f_{exp}(E_{il}, \theta_l)} \right)^2 \right],$$

where L is the number of emission angles, $\sum M_l$ is the number of data points for all angles. Conservation of two integral quantities (for the normalized spectra they are a number of emitted particles, $\langle N^{out} \rangle = 1$, and mean kinetic energy carried away by a single secondary particle, $\langle E^{out} \rangle$) has been taken into consideration by means of minimization of the following function:

$$F_2 = F_1 + S \cdot \left[\left(1 - \frac{\langle N^{out} \rangle}{\langle N_{exp}^{out} \rangle} \right)^2 + \left(1 - \frac{\langle E^{out} \rangle}{\langle E_{exp}^{out} \rangle} \right)^2 \right],$$

$$S = \sum_{l=1}^L \sum_{i=1}^{M_l} \frac{1}{W_{il}^2}.$$

The quantity $\langle E_{exp}^{out} \rangle$ is assumed to be known from theoretical models. However we have taken it from the D2N2+EVAP code calculation. Our choice of $\langle E_{exp}^{out} \rangle$ gives an opportunity to compare the transformation spectrum with Sychev's e.a.(1979) data being self-consistent by energy. Unfortunately the initial experimental data of thin lead target have been inaccessible for us. For this reason we use evaluated data from the ENDF/HE¹⁰.

Results of our fit by various minimization functions are shown in Fig.6. Values of a_{ni} and t_{ni} parameters derived through F_1 and F_2 minimization are in Table 3. F_2 -minimization spectrum as follows from Fig.6 has smaller deviation from D2N2+EVAP data at high energy region in comparison with F_1 -minimization one. But the former has a larger discrepancy at low emission energies. One can assume that the F_2 -minimization spectrum will be more accurate at low energies when more reliable statistical weights of data will be used for minimization.

Conclusions

The experience of the SITHA code exploitation showed us great capabilities of the "inclusive" approach. The future of this approach is connected with the development a reliable approximation of double differential spectra of emitted nucleons by modification of one of the well-known systematics or by creation of a new one. We supposed to include integral quantities during data set fitting. We believe it should be made by including the integral quantities, discussed here, during data set fitting.

References

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Table 1. Contents of the GR175-V1 library

Z	Sym.	A	MAT	N _{bands}	N _{words}	Z	Sym.	A	MAT	N _{bands}	N _{words}
1	H	1	8401	2	704	22	Ti	0	8428	5	2695
2	He	3	8404	3	1680	26	Fe	0	8432	4	2940
2	He	4	8405	1	1341	29	Cu	0	8438	3	2955
4	Be	7	8408	3	1453	31	Ga	0	8440	3	2713
4	Be	9	8909	2	2433	41	Nb	93	8443	5	3538
6	C	12	8412	3	3085	73	Ta	181	8455	5	4270
7	N	14	8413	2	3583	82	Pb	0	8462	2	2969
8	O	16	8414	4	2677	92	U	234	8467	2	3122
9	F	19	8415	3	4607	92	U	235	8468	5	4310
12	Mg	0	8417	3	3509	92	U	238	8471	5	4354
13	Al	27	8419	4	4007	94	Pu	240	8477	5	4575
14	Si	0	8420	4	2926	94	Pu	241	8478	3	3778
16	S	32	8422	3	2486	95	Am	241	8482	5	3792
17	Cl	0	8423	4	2966						

Table 2. Mean energy carried away by secondary particles from target T irradiated by projectiles Pr. Two approaches to double differential spectra representation are used: A –Sychev's e.a.(1979) model, B –ENDF/HE. Secondary particles are designated by n –neutrons, p –protons, π –mezon, LF –light fragment, E_b is binding energy. E_0 is energy of the projectile particle.

Pr	T		E_0	n	p	π	LF	E_b	E_{tot}
p	Pb	A	100	31.3	20.3	0	1.5	45.4	99.0
		B	100	89.4	30.6		0.1	41.5	161.6
		A	600	194.4	208.1	63.5	10.9	114.4	591.3
		B	600	457.1	297.8		12.1	104.4	871.0
n	Pb	A	100	38.0	14.2	0	1.5	45.4	99.1
		B	100	98.4	15.0		0.04	43.1	156.5
		A	600	284.2	118.2	63.0	10.9	114.4	590.7
		B	600	477.5	175.1		11.2	104.0	767.8
p	Fe	A	100	22.7	34.0	0	4.0	34.7	95.4
		B	100	23.1	39.9		4.2	34.9	102.1
		A	600	141.1	289.1	59.8	16.2	67.6	573.8
		B	600	286.6	339.3		27.4	76.4	729.7

Table 3. Results of fitting of ENDF/HE double differential spectra of emitted neutrons at reaction $p + Pb \rightarrow n + X$, $E_p = 600 \text{ MeV}$, by means of minimization of functions F_1 and F_2 .

Var.	n	a_{n0}	a_{n1}	a_{n2}	t_{n0}	t_{n1}	t_{n2}
F_1	1	1.1E-1	1.4E-2	1.2E-3	1.5E+0	-1.9E-1	5.5E-2
	2	1.2E-2	1.1E-2	7.7E-5	3.4E+0	-8.9E-1	4.9E-1
	3	1.4E-4	9.9E-5	2.7E-5	2.0E+1	-3.1E-1	1.8E+1
	4	1.4E-5	1.4E-5	5.6E-7	6.6E+1	1.7E+1	1.8E+1
F_2	1	1.4E-1	2.0E-2	7.7E-4	1.5E+0	-1.3E-1	4.0E-2
	2	1.1E-2	1.1E-2	1.2E-3	3.2E+0	-6.6E-1	4.3E-1
	3	1.3E-4	9.4E-5	5.4E-5	1.7E+1	-3.8E-1	3.2E+0
	4	4.1E-6	4.1E-6	9.6E-6	7.4E+1	1.6E+1	1.5E+1

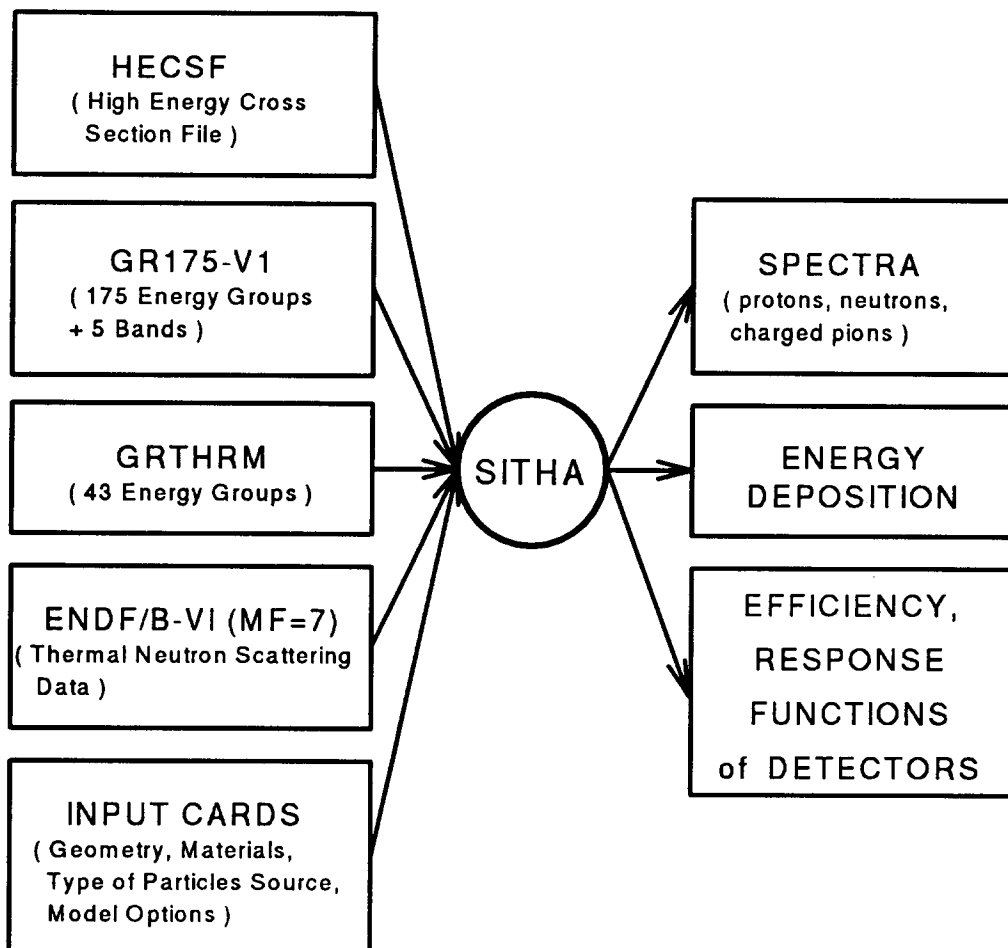


Fig. 1. Schematic representation of the SITHA code input and output possibilities.

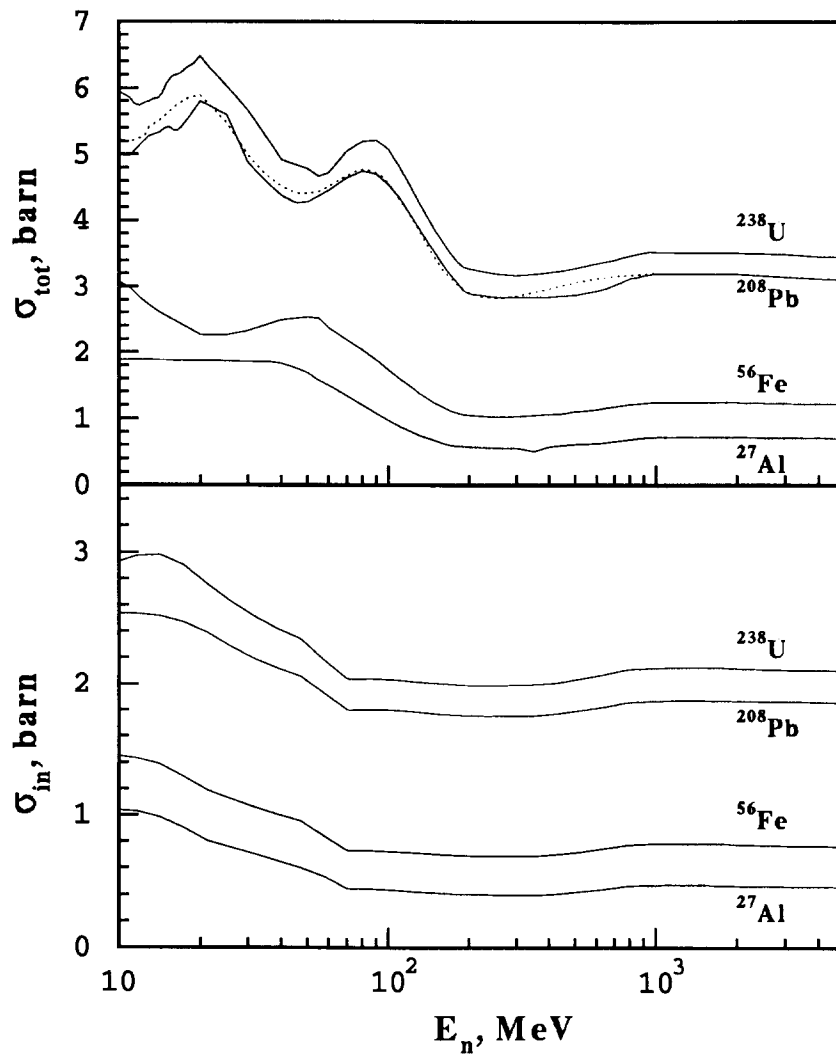


Fig. 2. The neutron total and inelastic cross sections from HECSE. The dashed line is from ENDF/HE.

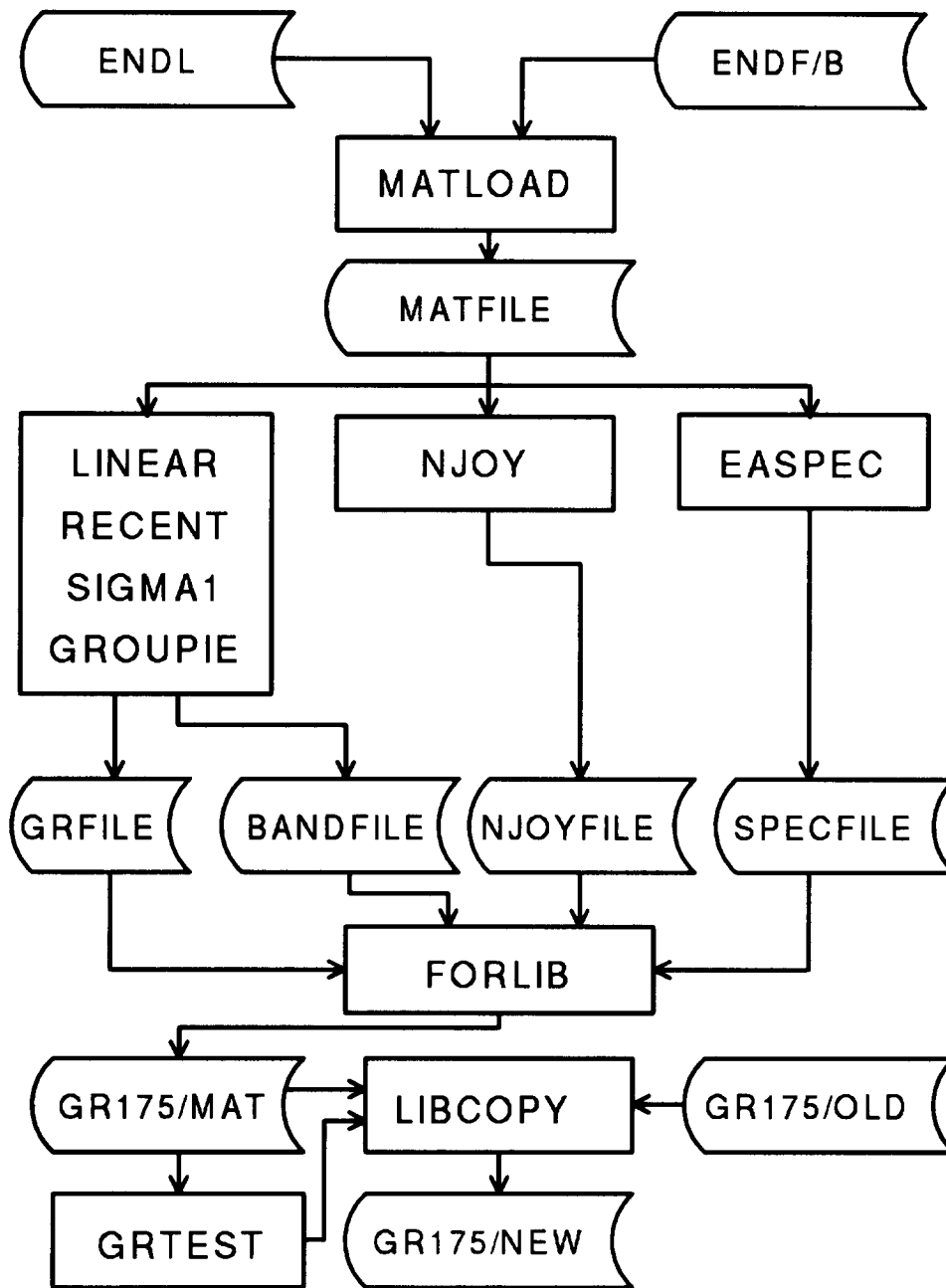


Fig. 3. Schematic illustration of the multigroup cross section preparation.

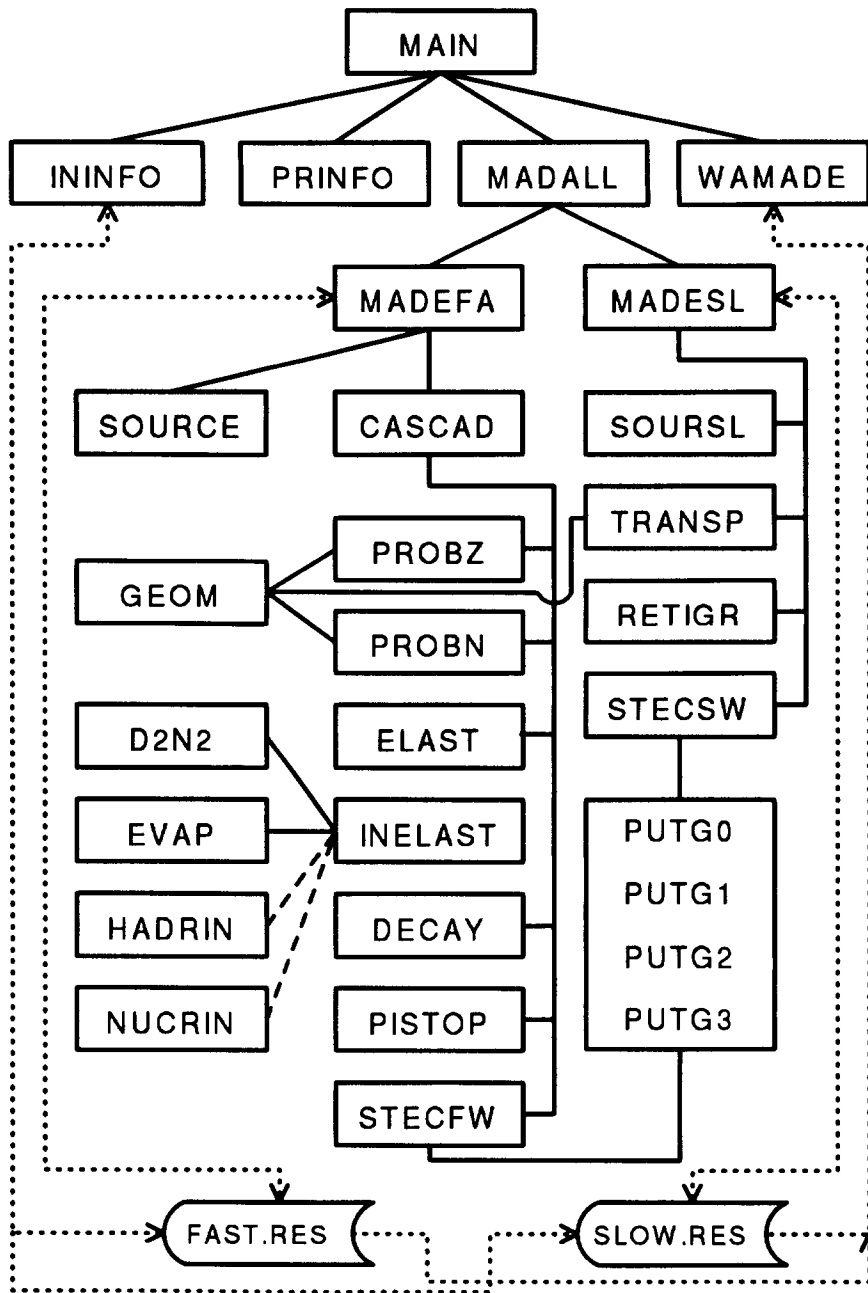


Fig. 4. Schematic illustration of the main subroutines structure of the SITHA code.

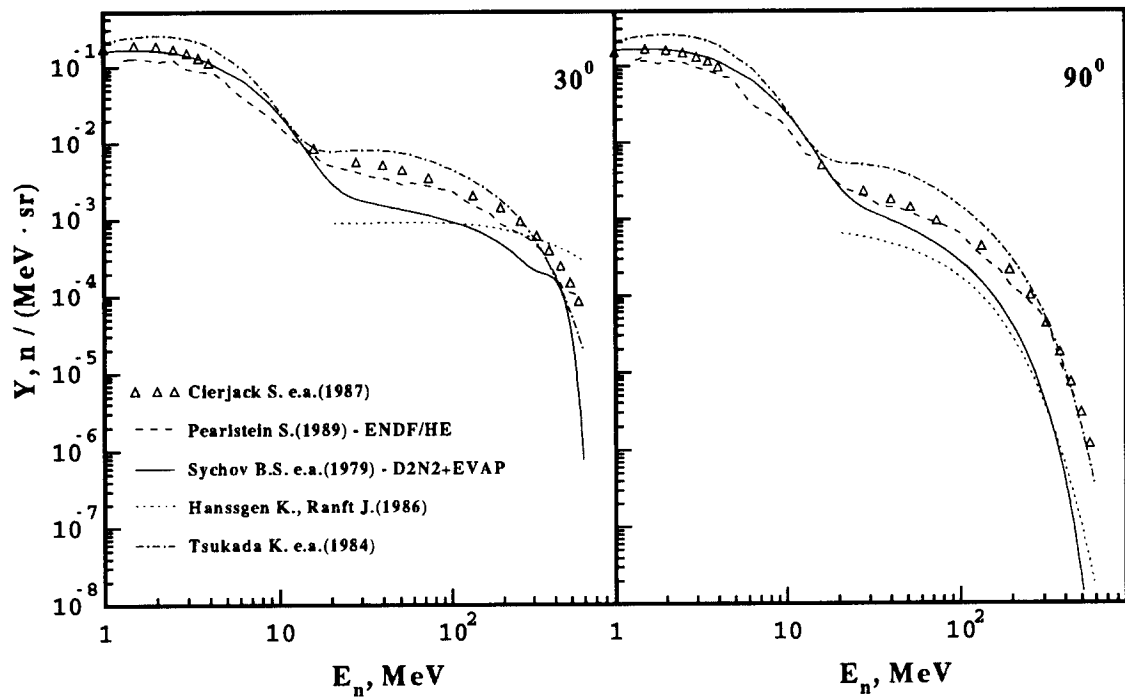


Fig. 5. The neutron emission spectra from a thin Pb target bombarded by 590 MeV protons and different approximations of them.

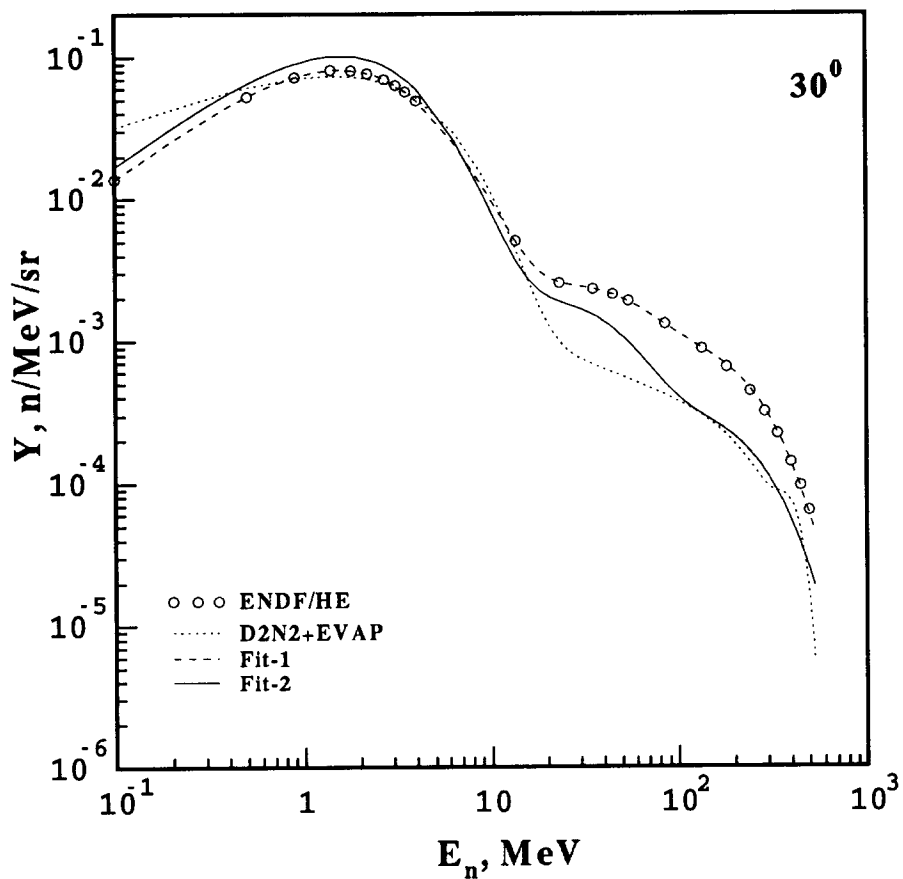


Fig. 6. Double differential neutron spectra of $p + Pb \rightarrow n + X$ reaction in different approximations ($E_p = 600$ MeV).

