

International Nuclear Model Code Comparison Study
of the Spherical Optical Model for Charged Particles

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1. Introduction

Several intercomparisons /1,/2/ of computer codes used to calculate nuclear cross sections show general agreement but significant differences in detail. Since these codes embody the same mathematical functions and the intercomparisons use the same input parameters one would expect if the codes are indeed identical, that the results would be the same to a high degree of accuracy, limited only by the rounding errors of the computer used. For most practical purposes the differences between the codes tested in previous intercomparisons are not important. It is however desirable to identify and, where necessary, correct the sources of these differences because they may well cause significant effects when the program is used in other domains of parameter space or when the code is used as a subroutine in a more extended calculation.

This report is concerned with simple optical model calculations but it is planned to extend it to other calculations. In Section 2 we summarize the preliminary intercomparison and tabulate the results of calculations of proton and alpha-particle elastic scattering made with several different codes. Section 3 summarizes the possible reasons for the discrepancies that are found, and Section 4 presents the results of selected intercomparisons in which the codes are altered to bring them into close conformity. These results can therefore serve as a standard.

The optical model formalism is given by Hodgson /3/.

2. Preliminary Intercomparison

A series of test calculations for protons and alpha-particles scattered at 5, 10, 15 and 20 MeV from carbon 12, cobalt 59 and lead 208 was specified as described in Appendix 1 to this report. This specification was sent to several users of spherical optical model codes and the results obtained for the reaction cross sections are given in Tables I and II. Some characteristics of the codes used are given in Appendix 2.

Examination of these tables shows, as expected, that all the codes used are essentially correct and their accuracy is more than adequate for practical purposes. Closer examination, however, shows significant differences and these are the subject of the present report. In particular it is notable that the results obtained with JIB and SCAT-2 are nearly always in accord to three decimal places, and often to four. Other codes show quite marked deviations from the average results, such as ABACUS-2 for 5 MeV protons on carbon 12, SMOG for 5 MeV protons on lead 208 and SCAT for 5 MeV protons on cobalt 59. On the whole the consistency is better for the heavy nuclei than for the light and better for the alpha-particles than for protons; this is expected because these interactions are more dominated by the Coulomb field and hence less sensitive to the nuclear potential. This is satisfactory confirmation that the routines calculating the Coulomb functions are essentially correct.

3. Reasons for the Discrepancies

There are several possible causes for the discrepancies between the codes and these may conveniently be divided into two classes: (a) mathematical and (b) numerical:

(a) Mathematical Discrepancies

There are several mathematical parameters that control the numerical integration of the radial wave equation, in particular (i) the step length (ii) the number of partial waves and (iii) the matching radius. These parameters are usually set automatically within the code to values that are more than adequate to ensure the required accuracy. The step length may be chosen to correspond to about ten steps per unit of kr , the number of partial waves so that the contributions of the last two waves included in the calculation contribute less than $\delta = 10^{-3}$ to the scattering matrix element and the matching radius to exceed $R + n\alpha$ where n is about 10. The values of these parameters in the programs studied in this exercise are given in Table III. Tests showed that in all cases these values were adequate, and so the observed discrepancies cannot be attributed to these choices.

(b) Numerical Discrepancies

There are two combinations of fundamental constants that enter the calculation, namely those used to obtain the wave number and the Coulomb parameter, and these are also included in Table III. The parameters specifying the potential must obviously be the same, but even here there is one possible source of discrepancy, namely rounding errors evaluating the potential depths from the formulae given; this applies only to the proton calculations.

4. Precision Calculations

The calculations were rerun with three codes altered so as to have exactly the same numerical and output parameters; the results are compared in Table IV. In Table V we also present the results of exactly similar calculations to those in Table IV but with the charge of the incident particle set to zero. This can serve as a standard to check neutron optical model calculations.

For the precision calculations the following parameters were used for C^{12} :

E	V_R	W_V	W_{SF}	a_I	l_{max}
5	53.4	0.0	10.6	0.51	9
10	51.8	0.0	9.3	0.51	10
15	50.2	0.6	8.1	0.51	12
20	48.6	1.7	6.8	0.51	13

The other parameters are energy and mass independent and are given below:

$r_R = 1.17$ fm	Wave number = 0.218732
$a_R = 0.75$ fm	Coulomb parameter = 0.157484
$r_I = 1.32$ fm	Total number of steps = 122
$V_{so} = 6.2$ MeV	Partial wave cut-off criterion = 10^{-6}
$r_{so} = 1.01$ fm	Matching radius $n \approx 10$
$a_{so} = 0.75$ fm	
$r_c = 1.25$ fm	

In addition, the SMOG program was run on two different computers using the same word length (32 bits) for storing data, namely IBM and VAX. These two computers store data internally in a different way. The results obtained from these calculations are also shown in Tables IVa, IVb, Va and Vb. The observed discrepancies give an indication of the maximum agreement one can expect in this kind of comparison. SMOG was then rerun in double precision on both computers and the agreement improved by three decimal figures. The results obtained on VAX in single precision appeared to be more accurate than those obtained with IBM. Table VI shows the average fractional deviation of the results obtained with an IBM as compared to VAX both in single and double precision for the proton as incident particle.

5. Conclusion

The comparisons made in this report show the accuracy that is presently attainable with optical model calculations. They also provide benchmarks that can be used to check any optical model program before it is used to analyse experimental data.

REFERENCES

- /1/ E. Sartori, Report on the International Nuclear Model Code Intercomparison, Coupled Channel Model Study, NEANDC-182A-INDC(NEA)3, 1984.
- /2/ A. Prince, G. Reffo and E. Sartori, Report on the International Nuclear Model Code Intercomparison Spherical Optical and Statistical Model Study, NEANDC-152A-INDC(NEA)4, 1983.
- /3/ P.E. Hodgson, The Optical Model of Elastic Scattering, Oxford University Press, 1963.

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Table Ia - Incident Particle: Proton

Reaction Cross Section (m barn)

E(lab) (MeV)	SCAT	ABACUS-2	ELIESE-3	SMOG	JIB	SCAT-2
C^{12}						
5	807.20	802.59	810.94	811.48	811.27	810.65
10	751.48	752.79	753.52	749.97	749.56	749.56
15	679.50	680.90	681.91	678.07	677.72	677.82
20	602.05	602.38	608.35	602.03	601.91	601.91
Ca^{59}						
5	371.83	372.41	372.49	372.45	372.45	372.48
10	939.99	940.56	941.95	942.17	941.74	941.39
15	1128.47	1128.6	1126.9	1126.72	1126.54	1126.86
20	1185.14	1186.1	1188.0	1188.34	1188.09	1187.88
Pb^{208}						
5	0.0864	0.0925	0.0909	0.0478	0.091	0.0925
10	188.14	190.79	190.38	189.80	190.61	190.76
15	932.35	933.60	933.13	932.61	933.52	933.70
20	1446.69	1450.7	1449.9	1449.45	1450.34	1450.48

Table Ib - Incident Particle: Proton; Target C¹²Shape Elastic Differential Cross Section (m barn/sterad)

Angle Degrees (C.M.)	ABACUS-2	ELIESE-3	SMOG	JIB	SCAT-2
$E(\text{lab}) \approx 5 \text{ MeV}$					
10	33863.	33801.	33798.	33803.	33806.
50	85.21	85.66	85.39	85.57	85.56
90	5.802	5.570	5.39	5.389	5.435
130	15.97	15.61	15.70	15.57	15.73
170	21.06	22.30	22.59	22.66	22.47
$E(\text{lab}) = 10 \text{ MeV}$					
10	7642.	7634.	7628.	7634.	7633.
50	49.68	50.06	51.15	51.33	51.26
90	15.20	15.28	15.50	15.48	15.44
130	9.454	8.463	8.65	8.63	8.673
170	4.132	5.263	5.67	5.639	5.526
$E(\text{lab}) = 15 \text{ MeV}$					
10	3300.	3283.	3259.	3263.	3263.
50	40.47	40.70	42.05	42.16	42.07
90	18.56	18.17	18.08	18.02	18.03
130	3.157	2.734	2.79	2.783	2.796
170	3.353	4.550	4.64	4.663	4.637
$E(\text{lab}) = 20 \text{ MeV}$					
10	1984.	1973.	1943.	1945.	1946.
50	34.65	34.32	35.30	35.39	35.38
90	12.92	12.51	12.56	12.54	12.55
130	1.248	0.9899	1.01	1.006	1.017
170	1.507	2.091	2.22	2.218	2.214

Table Ic - Incident Particle : Protons Target C¹²

Polarizations

Angle Degrees (C.M.)	ABACUS-2	ELIESE-3	SMOG	JIB	SCAT-2
E(lab) = 5 MeV					
10	- 0.0012	0.0008	0.001	0.0008	0.0008
50	0.0088	- 0.0470	- 0.046	- 0.0473	- 0.0482
90	- 0.4868	0.5144	0.516	0.5146	0.5236
130	- 0.4146	0.3415	0.340	0.3396	0.3462
170	- 0.1462	0.1174	0.116	0.1155	0.1183
E(lab) = 10 MeV					
10	- 0.0075	0.0028	0.003	0.0028	0.0029
50	0.1666	- 0.2344	- 0.234	- 0.2350	- 0.2398
90	- 0.3910	0.2668	0.264	0.2613	0.2685
130	0.1081	- 0.0920	- 0.087	- 0.0846	- 0.0850
170	- 0.6035	0.4216	0.408	0.4091	0.4205
E(lab) = 15 MeV					
10	- 0.0354	0.0172	0.017	0.0174	0.0178
50	0.1646	- 0.2610	- 0.249	- 0.2498	- 0.2550
90	- 0.3625	0.2973	0.292	0.2892	0.2957
130	0.1873	- 0.0710	- 0.077	- 0.0767	- 0.0737
170	- 0.5121	0.3473	0.344	0.3437	0.3477
E(lab) = 20 MeV					
10	- 0.0073	0.0345	0.035	0.0353	0.0361
50	0.1266	- 0.1993	- 0.186	- 0.1879	- 0.1911
90	- 0.2911	0.2706	0.276	0.2748	0.2811
130	- 0.5642	0.6673	0.630	0.6329	0.6451
170	- 0.5427	0.3807	0.376	0.3755	0.3786

Table II - Incident Particle : Alpha

Reaction Cross Section (m barn)

E(lab) (MeV)	SCAT	ABACUS-2	ELIESE-3	SMOG	JIB	SCAT-2
C^{12}						
5	504.56	505.03	504.85	504.57	504.96	505.00
10	820.79	821.25	821.40	821.13	821.16	821.19
15	886.75	887.19	887.25	886.93	887.15	887.16
20	907.18	908.21	908.26	907.91	908.19	908.21
Co^{59}						
5	0.0430	0.0163	0.0159	0.0210	0.016	0.0163
10	252.95	248.59	248.52	248.03	248.54	248.58
15	847.91	848.94	848.74	848.44	848.92	848.94
20	1144.65	1145.7	1145.5	1145.16	1145.68	1145.71
Pb^{208}						
15		0.0908	0.0795	0.0611	0.086	0.0908
20		84.775	84.610	84.204	84.75	84.779

Table III - Values of Parameters of Codes

Parameter Code	Total Number of Steps	Partial Wave Cut-off	Matching Radius n	Wave Number	Coulomb Parameter
SCAT			7	0.21729	
ABACUS-2	varying with energy \leq 500	varying with energy 10^{-6} - 10^{-9}	parameter given in input 4, 5, 6 or 7	0.21873427	0.1574860
ELIESE-3	varying	varying	\approx 10	0.2187342	0.1574862
SMOG	150	10^{-4}	10	0.2187342	0.1574862
JIB	122	10^{-7}	\approx 13	0.218732	0.157484
SCAT-2	200	10^{-6}	\approx 13	0.21873427	0.1574860

Table IVa - Incident Particle: Proton; Target C¹²

Shape Elastic Differential Cross Section (m barn/sterad)

Reaction Cross Section (m barn)

C¹²

Angle Degrees (C.M.)	SMDG			JIB (VAX)	SCAT-2 (CDC)
	(IBM-VAX)		(VAX)		
	Double P.	Single P.	Single P.		
E(lab) ≈ 5 MeV					
σ _r	811.14	811.14	811.33	811.16	810.58
10	33809.	33809.	33802.	33805.	33813.
50	85.83	85.83	85.70	85.84	85.84
90	5.400	5.400	5.388	5.374	5.418
130	15.65	15.65	15.64	15.66	15.65
170	22.52	22.52	22.48	22.52	22.33
E(lab) ≈ 10 MeV					
σ _r	749.62	749.62	749.80	749.59	749.47
10	7635.	7635.	7629.	7634.	7636.
50	51.31	51.32	51.29	51.51	51.43
90	15.45	15.45	15.46	15.44	15.40
130	8.657	8.657	8.662	8.633	8.678
170	5.609	5.609	5.626	5.605	5.488
E(lab) ≈ 15 MeV					
σ _r	679.83	679.83	680.01	678.90	678.98
10	3269.	3269.	3267.	3263.	3265.
50	41.91	41.91	41.90	42.05	41.98
90	18.05	18.05	18.06	17.89	17.89
130	2.762	2.762	2.767	2.732	2.743
170	4.555	4.555	4.556	4.576	4.547
E(lab) ≈ 20 MeV					
σ _r	604.19	604.19	604.23	601.79	601.78
10	1960.	1960.	1959.	1944.	1945.
50	35.55	35.55	35.55	35.43	35.43
90	12.69	12.69	12.69	12.51	12.52
130	1.044	1.044	1.046	0.999	1.010
170	2.136	2.136	2.139	2.209	2.209

Table IVb - Incident Particle: Proton; Target C¹²Polarization

Angle Degrees (C.M.)	SMOG			JIB (VAX)	SCAT-2 (CDC)
	(IBM-VAX) Double P.	(VAX) Single P.	(IBM) Single P.		
E(lab) = 5 MeV					
10	0.0008	0.0008	0.0008	0.0008	0.0008
50	- 0.0464	- 0.0464	- 0.0459	- 0.0466	- 0.0475
90	0.5139	0.5139	0.5147	0.5142	0.5233
130	0.3395	0.3395	0.3390	0.3385	0.3455
170	0.1151	0.1151	0.1151	0.1148	0.1176
E(lab) = 10 MeV					
10	0.0028	0.0028	0.0028	0.0028	0.0029
50	- 0.2349	- 0.2349	- 0.2341	- 0.2347	- 0.2395
90	0.2621	0.2621	0.2638	0.2620	0.2693
130	- 0.0831	- 0.0831	- 0.0848	- 0.0835	- 0.0836
170	0.4103	0.4103	0.4096	0.4096	0.4212
E(lab) = 15 MeV					
10	0.0173	0.0173	0.0173	0.0174	0.0178
50	- 0.2516	- 0.2516	- 0.2506	- 0.2494	- 0.2543
90	0.2888	0.2888	0.2903	0.2898	0.2965
130	- 0.0710	- 0.0710	- 0.0718	- 0.0780	- 0.0748
170	0.3454	0.3455	0.3441	0.3420	0.3460
E(lab) = 20 MeV					
10	0.0349	0.0349	0.0349	0.0353	0.0361
50	- 0.1880	- 0.1880	- 0.1872	- 0.1877	- 0.1908
90	0.2725	0.2725	0.2739	0.2758	0.2819
130	0.6340	0.6340	0.6332	0.6336	0.6450
170	0.3813	0.3812	0.3824	0.3747	0.3776

Table Va - Incident Particle: Neutron; Target C¹²Shape Elastic Differential Cross Section (m barn/sterad)Reaction Cross Section (m barn)

Angle Degrees (C.M.)	SMOG			JIB (VAX)	SCAT-2 (CDC)
	(IBM-VAX)		(IBM)		
	Double P.	Single P.	Single P.		
E(lab) = 5 MeV					
$\frac{\sigma_{SE}}{\sigma_r}$	526.00 1082.32	526.00 1082.32	525.76 1082.62	525.86 1082.25	1081.55
10	319.4	319.4	319.2	319.2	318.9
50	60.20	60.20	60.18	60.18	60.18
90	5.747	5.746	5.736	5.760	5.745
130	14.31	14.31	14.30	14.32	14.38
170	25.73	25.73	25.78	25.69	25.43
E(lab = 10 MeV					
$\frac{\sigma_{SE}}{\sigma_r}$	676.15 871.56	676.15 871.56	676.00 871.65	677.29 871.47	871.66
10	563.4	563.4	563.3	564.2	563.9
50	40.67	40.67	40.68	40.88	40.78
90	23.06	23.06	23.07	23.04	23.01
130	8.781	8.781	8.765	8.763	8.813
170	11.90	11.90	11.90	11.88	11.72
E(lab) = 15 MeV					
$\frac{\sigma_{SE}}{\sigma_r}$	859.24 748.53	859.24 748.53	859.15 748.52	857.27 747.62	747.60
10	885.2	885.2	885.1	882.4	881.4
50	42.77	42.77	42.77	42.84	42.79
90	22.37	22.37	22.37	22.19	22.21
130	3.251	3.251	3.251	3.203	3.217
170	6.386	6.387	6.381	6.420	6.370
E(lab) = 20 MeV					
$\frac{\sigma_{SE}}{\sigma_r}$	950.19 645.57	950.18 645.57	950.27 645.53	940.21 643.30	643.26
10	1152.	1152.	1152.	1136.	1135.
50	43.18	43.18	43.17	42.82	42.85
90	14.29	14.29	14.29	14.13	14.13
130	1.741	1.741	1.741	1.695	1.707
170	2.124	2.124	2.127	2.199	2.199

Table Vb - Incident Particle: Neutron; Target C¹²

Polarization

Angle Degrees (C.M.)	SMOG			JIB (VAX)	SCAT-2 (CDC)
	(IBM-VAX) Double P.	(VAX) Single P.	(IBM) Single P.		
E(lab) = 5 MeV					
10	- 0.0089	- 0.0089	- 0.0091	- 0.0089	- 0.0091
50	- 0.0681	- 0.0681	- 0.0681	- 0.0688	- 0.0699
90	0.1423	0.1423	0.1400	0.1420	0.1487
130	0.1619	0.1619	0.1614	0.1608	0.1641
170	0.1782	0.1783	0.1771	0.1780	0.1825
E(lab) = 10 MeV					
10	- 0.0028	- 0.0028	- 0.0032	- 0.0028	- 0.0030
50	- 0.2473	- 0.2473	- 0.2477	- 0.2470	- 0.2524
90	0.2013	0.2012	0.2000	0.2013	0.2064
130	- 0.1491	- 0.1491	- 0.1493	- 0.1496	- 0.1498
170	0.3526	0.3526	0.3534	0.3521	0.3603
E(lab) = 15 MeV					
10	- 0.0113	- 0.0113	- 0.0115	- 0.0111	- 0.0114
50	- 0.2197	- 0.2197	- 0.2197	- 0.2186	- 0.2230
90	0.2011	0.2011	0.2010	0.2019	0.2065
130	0.1933	0.1932	0.1941	0.1876	0.1956
170	0.3701	0.3700	0.3705	0.3669	0.3724
E(lab) = 20 MeV					
10	- 0.0101	- 0.0101	- 0.0103	- 0.0095	- 0.0097
50	- 0.1176	- 0.1176	- 0.1174	- 0.1195	- 0.1212
90	0.2190	0.2190	0.2194	0.2215	0.2269
130	0.6878	0.6878	0.6886	0.6831	0.6959
170	0.4429	0.4429	0.4408	0.4353	0.4383

Table VI - Comparison of SMOC on IBM and VAX for $\alpha + C^{12}$

Average Fractional Deviation (*)

a) Single Precision (10^{-3})

Energy	Differential Cross Section	Polarization
5	1.4	7.5
10	1.2	56.
15	0.9	8.2
20	0.8	4.3

b) Double Precision (10^{-5})

Energy	Differential Cross Section	Polarization
5	1.2	2.7
10	1.9	93.
15	1.8	7.1
20	1.6	2.4

(*) The averages were calculated over 36 angles at intervals of 5 degrees. However, these averages depend on the choice of the angular mesh.

Appendix 1

Definition of Optical Potential

(according to Becchetti & Greenlees, Phys. Rev. 182, 1190 (1969))

<u>Expression</u>	<u>Validity Range</u>	<u>Explanation</u>
$U_{\text{opt}}(r) = -V_R f_R$		central real
$+ \left(\frac{\pi}{m_\pi c} \right)^2 \frac{v_{\text{so}}}{r} \left(\frac{d}{dr} f_{\text{so}} \right) \vec{l} \cdot \vec{\sigma}$		spin orbit
$\left\{ \frac{Zze^2}{2R_c} \left[3 - \left(\frac{r}{R_c} \right)^2 \right] \right.$	for $r \leq R_c$	
$+ \left\{ \frac{Zze^2}{r} \right.$	for $r \geq R_c$	Coulomb
$- iW_V f_I$		imaginary volume
$+ i4a_I W_{SF} \frac{d}{dr} f_I$		imaginary surface

$$\text{where } f_X = f(r, R_X, a_X) = [1 + \exp(r - R_X)/a_X]^{-1}$$

$$R_X = r_X^{A/3}$$

r_c = Coulomb radius

Note: Whenever a parameter is omitted, it is assumed that the corresponding potential is not considered.

Proton Parameters: Becchetti & Greenlees, Phys. Rev. 182, 1190 (1969)

$$V_R = 54.0 - 0.32E + 0.4Z/A^{1/3} + 24.0(N - Z)/A \text{ MeV}$$

$$r_R = 1.17 \text{ fm}$$

$$a_R = 0.75 \text{ fm}$$

$$W_V = 0.22E - 2.7 \text{ or zero, whichever is greater}$$

$$W_{SF} = 11.8 - 0.25E + 12.0(N - Z)/A \text{ MeV or zero, whichever is greater}$$

$$r_I = 1.32 \text{ fm}$$

$$a_I = 0.51 + 0.7(N - Z)/A \text{ fm}$$

$$V_{SO} = 6.2 \text{ MeV}$$

$$r_{SO} = 1.01 \text{ fm}$$

$$a_{SO} = 0.75 \text{ fm}$$

$$r_c = 1.25 \text{ fm}$$

Alpha Parameters: McFadden & Satchler, Nucl. Phys. 84, 177 (1966)

$$V_R = 164.7 \text{ MeV}$$

$$r_R = 1.442 \text{ fm}$$

$$a_R = 0.520 \text{ fm}$$

$$W_V = 22.4 \text{ MeV}$$

$$r_I = r_R$$

$$a_I = a_R$$

$$r_c = 1.25 \text{ fm}$$

Appendix 2

Computer Codes Used

<u>Name</u>	<u>Reference/Author</u>	<u>Participant</u>
SCAT	W.R. Smith, Comp. Phys. Comm. 1/1969/106 "Nuclear Penetrability and Phase Shift Subroutine"	M. Herman IBJ, Warsaw, Poland
ABACUS-2	E.H. Auerbach, BNL-6592 (1964)	B.V. Carlson M.P. Isidro R.A. Rego IEAV-CTA, San José dos Campos, Brazil
ELIESE-3	S. Igarashi, JAERI-1224 (1972) "A Program for Calculation of the Nuclear Cross-Sections by Using Local and Non-Local Optical Models and Statistical Model"	S.B. Garg Amar Sinha BARC, Trombay, India
SMOG	F. Fabbri, CEC/63-61-S0-04 (1963) Un Programma per il Calcolo dei Parametri di Interazione Neutron- Nucleo con il Modello Ottico"	F. Fabbri ENEA, Bologna, Italy
JIB	F.G. Perey Oak Ridge National Laboratory Oak Ridge, USA	P.E. Hodgson Nuclear Physics Laboratory University of Oxford, U.K.
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