Getting started with FRESCO

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1 General structure

FRESCO is a general-purpose reaction code, created and frequently updated by Ian Thompson. The code calculates virtually any nuclear reaction which can be expressed in a coupled-channel form. There is a public version of the code which can be downloaded from the website www.fresco.org.uk. FRESCO is accompanied by SFRESCO, a wrapper code that calls FRESCO for data fitting, SUMBINS and SUMXEN, two auxiliary codes for integrated cross sections. Although we do not include it here, in the same site you can also find XFRESCO the front-end program to FRESCO for X-window displays.

Its original version was written in Fortran 77 but some important sections were ported to Fortran 90. An important part concerns the input, which now uses *namelist* format, making it much easier to view the relevant variables. In this section we will discuss the general namelist format of the FRESCO input.

There are several different layers of output produced by FRESCO. The default output contains the most important information concerning the calculation, repeating the input information, and the resulting observables but most detailed information is contained in the generated fort files, including files ready for plotting purposes. At the end of this section we present the list of output produced by FRESCO.

1.1 Input file

Input files contain five major namelists regarding different aspects of the calculation: *fresco, partition, pot, overlap, coupling*. The first is for general parameters, the second for defining the properties intrinsic to the projectile and the target, the third for potentials, the fourth for the radial overlap functions and the last for the couplings to be included. Keep in mind that in some inputs, you may not find all these namelists. As FRESCO can calculate rather intricate processes, input files can sometimes look daunting. However, with the namelist format, you do not need to define all variables but only those that are relevant for your example. Below we introduce the contents of each namelist and their purpose. Detailed instructions are given in the FRESCO input manual on the website.

heading

Every input file starts with a heading (80 characters) that should describe and identify the reaction to be calculated, with perhaps some detail of the method and states included. The following line begins with NAMELIST

to indicate the subsequent style of input.

&fresco

This section introduces the parameters involved in the numerical calculations. It contains the radial information: the step with which the coupled-channel equations are integrated (*hcm*) and the radius at which the integrated wave function gets matched to the asymptotic form (*rmatch*). Whenever non-local kernels are involved a few more parameters are needed, (*rintp, hnl, rnl, centre*), but these will be discussed in subsection 2.4.[1]

In this namelist you also find general options for the calculations and the desired observables. Cross sections are calculated from the angular range *thmin–thmax* (in degrees) in steps of *thinc*. This is also where you define the number of partial waves in the calculation, by providing the initial and final total angular momentum: *jtmin, jtmax*.[2]

absend controls the convergence. If in the interval max(0,*jtmin*) $<$ J $<$ *jtmax* the absorption in the elastic channel is smaller than *absend* mb for three consecutive $J\pi$ sets, the calculation stops. When *absend*< 0, it takes the full J-interval.[3]

There are many control variables which trace intermediate steps in the calculation (starting from zero, increasing values will give more in depth information). Here we shall mention just a few of the most frequently used. For printing the coupled partial waves for each J^π (total angular momentum and parity) use *chans*; for details of the coupling coefficients *listcc*, and for S matrices use *smats* (absorption & reaction cross sections for successive partitions and excitations are output when *smats*≥ 1, and elastic S-matrix elements are ouput when *smats*≥ 2). The variable *xstabl*>0 prints the cross sections and tensor analyzing powers up to rank *k=xstabl* for all excitation levels in all partitions in Fortran file 16 (usually called fort.16).

Finally, and most importantly, this is the place where the beam energy is specified through *elab*. If you want a calculation at several energies, you can use the array *elab(i) i=1,4* and *nlab(i), i=1,3* to define the boundary points and the number of intermediate energy steps between *elab(i)* and *elab(i+1)*.

By default, the code assumes the elastic channel, the channel with the incoming plane wave, is the first excitation of the first partition. You can change this by using *pel>1* for the partition number and *exl>1* for the excitation within that partition. Also, *elab* refers by default to the energy of the projectile *lin*=1, but you can easily change the calculation to inverse kinematics by setting *lin*=2.

&partition

In *partition* you introduce all the mass partitions and the corresponding channels to be considered in the reaction. In the simplest case, elastic scattering within the optical model, you introduce just one partition, including the details of the projectile (*namep, massp, zp*) and the details of the target (*namet, masst, zt*). The Q-value for the reaction is given with *qval* (MeV) and the number of states that you want to include in this partition is *nex*.

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[1]It is often useful to introduce lower radial cutoffs in the calculations, especially for scattering below the Coulomb barrier. With *cutr* (fm) or *cutl* you introduce a lower radial cutoff in the coupled-channel equations. Whereas *cutr* is the same for all partial waves, *cutl* allows you to define an *L*-dependent cutoff (*L* is the total angular momentum of the set). The code will use max(*cutl*L*hcm,cutr*). If *cutr* is negative, the lower cutoff is put at that distance inside the Coulomb turning point. Finally, *cutc* (fm) removes off-diagonal couplings inside the given radius.

[2]To enable greater speed and flexibility, you can define a number of angular momentum intervals *jump(i), i=2,5* and the steps with which you want to perform the calculation *jbord(i), i=2,5*. Note that *jump(1)*=1 and *jbord(1)=jtmin*, so that the first interval is calculated fully. The omitted J values are provided by interpolation on the scattering amplitudes $A(m'M' : mM;L)$ prior to calculating cross sections. *jsets* is a variable that enables the calculation of positive parity (*jsets*='P') or negative parity only (*jsets*='M' or 'N'), for each energy. If *jsets*= 0, ' ', or F, no restriction is made.

[3]Sometimes, for accurate elastic-scattering cross sections it is only necessary to include the elastic channel. This can be done with the option *jtmin*<0. Then, in the range $J <$ abs(*jtmin*), transfers and excited states are ignored in the calculation.

Below defining each partition, you have to introduce the *nex* associated pairs of states (at least one). This is done through another namelist &*states*.

&*states*

Each pair of states is a specific combination of one state of the projectile and one state of the target. So this is the place where you introduce the spin, parity and excitation energy of these states: (*jp, ptyp, ep*) for projectile and (*jt, ptyt, et*) for target. The variables *bandp* and *bandt* are synonyms for *ptyp* and *ptyt* respectively. The optical potential for the distorted wave for $p + t$ relative motion is given by the index *cpot*, also defined here. This namelist is repeated as many times as necessary, to introduce all the pairs of states you wish to include in the calculation. When repeating the &*states* namelist, if one of the bodies stays in the same state, you should not introduce spin, parity and excitation energy again, but just set *copyp* or *copyt* to refer to the &*states* namelist in which the original state was first introduced.

&*pot*

This namelist contains the parameters for the potentials to be used in the reaction calculation, either for bound single-particle states or optical potentials. The namelist is repeated for each term in the potential. To identify the potential, there is an index *kp*, and all the components with a given *kp* value are added together to produce the potential used. So, when calculating the distorted waves, *cpot* will refer to one of the *kp*. The same will be used when calculating the bound single-particle states with *kbpot* (in &*overlap*). Each term in the potential is characterized by a type and a shape, followed by parameters *p(i), i* = 1,...,6. Traditionally, we define the Coulomb term first (*type*=0, *shape*=0 for a charged sphere). Then *p(1)=ap* and *p(2)=at* correspond to mass number of the projectile and the target needed for the conversion of the reduced radii into physical radii $R = r(ap^{1/3} + at^{1/3})$. The *p(3)=r_c* is the reduced Coulomb radius. Note that the same mass factor $(ap^{1/3} + at^{1/3})$ is used in all terms of a given potential. *type*=1 corresponds to the volume nuclear interaction, with *shape*=0 for Woods-Saxon shape.[4] The parameters for the real part are *p(1)=V_0*, *p(2)=r_0*, *p(3)=a_0* (for depth in MeV, the reduced radius in fm and the diffuseness in fm), while the parameters for the imaginary part are *p(4)=W_i*, *p(5)=r_i*, *p(6)=a_i*. A surface nuclear interaction is introduced with *type*=2 and the spin-orbit with *type*=3, for the projectile, and *type=4* for the target.[5]

When the potential does not have an analytic form, it is useful to read it in numerically. This can be achieved setting *shape*=7,8,9 to read from file fort.4 the real or the imaginary part of the potential, or the full complex potential, respectively.

&*overlap*

Overlap functions are needed in single-particle excitation calculations or in transfer calculations. The overlaps can refer to bound states and scattering states, but we will leave the latter for subsection 2.3. Every &*overlap* begins with an index *kn1*. The overlap function tells us how the composite nucleus B looks relative to its core A. The composite nucleus and the core are in partition *ic1* and *ic2* respectively, and refer to the projectile (*in*=1) or target (*in*=2). In the simpler case *kind*=0, we ignore the spin of the core and take $|(l, sn) j\rangle$ coupling.[6] The overlap has *nn* number of nodes (including the origin), *l* relative angular momentum, *sn* for the spin of the additional fragment (typically a neutron or proton *sn*=1/2), and total angular momentum *j*. The potential used in the calculation of the state is that indexed *kbpot*. You can also introduce the binding energy *be* if you want

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[4]A large number of standard shapes are predefined, of which we mention *shape*=2 for the Gaussian form $\exp[-(r-R_0)^2/b^2]$ (with $p(2)=r_0$ and $p(3)=b$) as the most common alternative.

[5]Tensor interactions and projectile/target deformation can be introduced with *type=5–11*. We will return to this in subsection 2.2.

[6]Multi-channel spin couplings are also available with *kind*=3.

the potential to be adjusted to reproduce the binding energy (*isc*=1 for adjusting the depth of the central part). If no rescaling is needed, set *isc*=0. A spectroscopic amplitude for the overlap can be set to the value $\sqrt{nam}*ampl$ if both of these are non-zero. This amplitude can also be introduced after &*coupling* in the namelist &*cfp*. For printing more detailed information into the standard output, there is a trace variable *ipc*. Its default value is zero, and, as it increases, it provides more detailed information on the overlap function.[7]

&*coupling*

Couplings are calculated with the information given in this namelist and include general spin transfer (*kind*=1); electromagnetic couplings (*kind*=2), single particle excitations (*kind*=3, 4 for projectile and target respectively); transfer couplings (*kind*=5, 6, 7, 8 for zero-range, local energy approximation, finite-range and non-orthogonality corrections respectively). The coupling is from all states in partition *icfrom* to all states in partition *icto*. Couplings are included in the reverse direction unless *icto* < 0. For specific options of the coupling we use the parameters *ip1, ip2, ip3* and for choices of the potentials in the operator there are *p1, p2* parameters. More detail on this namelist and others that follow will be given with specific examples.

1.2 Output files

The main output file (fort.6 or stdout) contains first of all a representation of all the parameters read from the input file. It will provide a summary of the calculation of the overlap functions (including binding energy, depth of the adjusted potential, rms radius and asymptotic normalization coefficient) and the coupling matrix elements. For each beam energy, it provides some information relative to the kinematic variables in the reaction followed by the contribution to the cross section of each partial wave. Integrated cross sections and angular distributions are printed at the end of the file.

Also at the end of the standard output file, as a reminder to the user, is a list of other files that were created during the run with additional information. Here we mention a few: fort.16 contains all angular distributions in a graphic format (to be read by XMGR or XMGRACE); fort.13 contains total cross sections for each channel; fort.56 contains the total absorptive, reaction and non-elastic cross section for each angular momentum. Separate cross sections are included in files 201, 202, etc., in the order they were specified. A full list of file allocations is given in Table 1.

2 Learning through examples

2.1 Elastic scattering

As an elastic scattering example, we chose the proton scattering on ^{78}Ni within the optical model. This exotic nucleus is an important waiting point in the r-process. The input for our example is shown Box 1. The calculations are performed up to a radius of *rmatch*=60 fm and partial waves up to *jtmax*=50 are included. Three beam energies are calculated. For this case, only one partition is needed with the appropriate ground states specified (the proton is spin 1/2 and positive parity, and the ^{78}Ni, being an even-even nucleus, has $J^{\pi} = 0^+$). The only remaining ingredient is the potential between the proton and ^{78}Ni (indexed *cpot=kp*=1) which contains a Coulomb part and a nuclear real and imaginary part. The results can be found in the standard output file, but it is easier to plot the fort.16 file to obtain Fig. 1.

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[7]Radial wave functions of bound states can be obtained by setting *ipc* odd, intermediate iterations with *ipc*≥3, and the final iteration with *ipc*>0.

Table 1: File allocation for the inputs and outputs for FRESCO.

File	Routines	Use
2	SFRESCO	search specification file
3	FREADF, FR	temporary namelist file
4	INTER	input external KIND=1,2 form factors
	POTENT	input external potentials
5		standard input
6		standard output
7	DISPX	S-matrix elements
13	FR	total cross sections for each Elab
16	CRISS	tables of cross sections
17	FR	output scattering waves
20–33	For users	(eg bound states, amplitudes)
34	POTENT	output potentials
35	FR	astrophysical S-factors for E_{cm}
36	CRISS	scattering Legendre coefficients
37	CRISS	scattering amplitudes
38	DISPX	cross sections for each $J\pi$
39	FR	2 cross sections for each E_{cm}
40	FR	all cross sections for each E_{lab}
41	SOURCE	source terms at each iteration
42	SOURCE	bin wave functions for each E
43	INFORM	bin phase shifts as k functions
44	INFORM	bin phase shifts as E functions
45	ERWIN	scattering phase shift as E functions
46	INFORM	ANC ratios & bound wave functions
47		reduced matrix elements
48	FR	misc log file
55	INFORM	Single-particle wave functions
56	FR	J fusion, reaction and nonelastic
57	FR	output CDCC amplitudes
58	INFORM	bound state wave functions
59	INFORM	bound state vertex functions
60-62	RMATRIX	trace of R-matrix calculations
66	INTER	KIND=1 nonlocal formfactor
71	FR	phase shifts as E_{lab} functions
75	FR	astrophysical S-factors for Elab
89	MULTIP	all coupling potentials
105	FCN	χ^2 progress during fitting
106	FCN	parameter snapshots during fitting
200	CRISS	elastic cross section if not fort.201
201-210	CRISS	cross sections (cf 16) of up to 10 states
301	CDCIN	new Fresco input
303	SFRESCO	input search file
304	SFRESCO	output plot file
305	CDCIN	new input from CDCC, col format
306	SFRESCO/FRXX0	input Fresco file
307	SFRESCO/FRXX0	initial Output Fresco file
308	SFRESCO/FRXX0	main Output Fresco file

```
p+Ni78 Coulomb and Nuclear;
NAMELIST
 &FRESCO hcm=0.1 rmatch=60
           jtmin=0.0 jtmax=50 absend= 0.0010
           thmin=0.00 thmax=180.00 thinc=1.00
           chans=1 smats=2  xstabl=1
           elab(1:3)=6.9 11.00 49.350  nlab(1:3)=1 1 /

 &PARTITION namep='p' massp=1.00 zp=1
              namet='Ni78' masst=78.0000 zt=28 qval=-0.000 nex=1  /
 &STATES jp=0.5 bandp=1 ep=0.0000 cpot=1 jt=0.0 bandt=1 et=0.0000  /
 &partition /

 &POT kp=1 ap=1.000 at=78.000 rc=1.2  /
 &POT kp=1 type=1 p1=40.00 p2=1.2 p3=0.65 p4=10.0 p5=1.2 p6=0.500  /
 &pot /
 &overlap /
 &coupling /
```

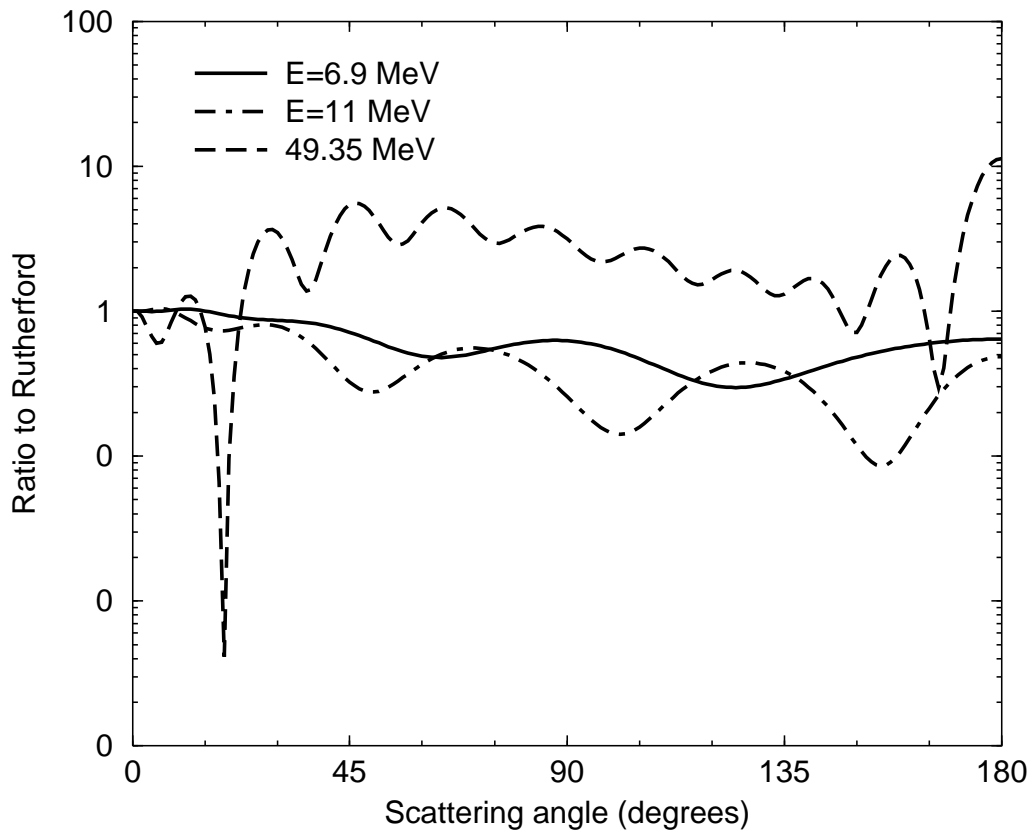Box 1: FRESCO input for the elastic scattering of protons on ^{78}Ni at several beam energies

Figure 1: Elastic scattering of protons on ^{78}Ni at several beam energies, calculated with input from Box 1.

2.2 Inelastic scattering

Inelastic scattering exciting collective states can be illustrated with the example $^{12}C(\alpha,\alpha)^{12}C(2^+)$, where the carbon nucleus gets excited into its first excited state. This reaction can provide complementary information to one of the most important reactions in astrophysics, the α-capture reaction on ^{12}C. In this type of inelastic reaction, only one partition is needed, but it contains two states. The projectile state is not changed (*copyp*=1) but the appropriate spin, parity and excitation energy need to be introduced for the target. The input is shown in Box 2.

In order for the reaction to happen, the potential needs to contain a tensor Y_{20} part to enable the target transition $0^+ \to 2^+$. This is done assuming a rotor model for the target and, in the input, only a deformation length needs to be introduced. For deforming a projectile *type*=10, while for deforming a target, *type*=11. Here the deformation length δ_2 is *p(2)*=1.3 fm, as twice highlighted in Box 2. The optical potential introduced includes a Coulomb term, the nuclear real term, and a nuclear imaginary with a volume (*type*=1) and a surface part (*type*=2). Each part needs to be deformed, and only the two nuclear parts are deformed. If Coulomb deformation were needed, an additional line after the Coulomb potential would have to be introduced with the same format, except that, instead of the deformation length, the reduced matrix element should be given.[8] As the proton and neutrons do not necessarily have the same spatial distribution, the deformation parameters will, in general, not be the same. The example shows a DWBA calculation as *iter*=1. You could check the validity of the DWBA by including higher-order terms in your Born expansion (increasing *iter*) or performing a full coupled-channels calculation (*iter*=0, *iblock*=2). Results for the inelastic excitation of ^{12}C are shown in Fig. 2

2.3 Breakup

Breakup calculations can be modeled as single-particle excitation into the continuum. In this example we show a typical CDCC calculation. It calculates the breakup of ^8B into p + ^7Be, under the field of ^{208}Pb at intermediate energies. The input is shown in Box 3. The breakup of ^8B has been measured many times with the aim of extracting the proton capture rate on ^7Be.

Several new ingredients need to be explained. First of all, due to the long range of the Coulomb interaction it is very important to include the effect of couplings out to large distances. Instead of integrating the CDCC equations up to very large radii, we introduce *rasym*. Setting *rmatch<0* tells the code that the integration of the equations should be done up to *rmatch*, numerically, but these should then be matched with coupled-channel Coulomb functions up to *rasym*. Also important are the partial waves. For these intermediate energies, many partial waves need to be included and it is useful, instead of calculating each single one, to interpolate between them. This can be done with *jump* and *jbord*. In this example, we start with *jtmin*=0 until $j = 200$ in steps of 1, for $jt = 200-300$ use steps of 10, for $jt = 300-1000$ use steps of 50, and for $jt = 1000-9000$ use steps of 200. With the inclusion of so many partial waves, the strong repulsion at short distances can introduce numerical problems. This is avoided with a radial cutoff $cutr = -20$ fm, where the minus sign puts the cutoff 20 fm inside the Coulomb turning point.

This example contains only *s*-waves in the continuum, sliced into 20 energy bins. Other partial waves (p, d, f are needed for convergence) are left out of this example to make it less time consuming (beware, it will still take a few minutes in a desktop computer!). Since in general there will be many channels involved, it is convenient to drop off channels/couplings whenever they are weak. This is done through *smallchan* and *smallcoup*. To perform a full CDCC calculation, *iter*=0 and *iblock*=21.

The continuum of ^8B is binned into discrete excited states of positive energy, so under the first partition the

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[8]If you do not want to assume a rotational model, you can introduce these couplings (either deformation length or matrix element) for each initial-to-final state through *type*=12, 13 for projectile and target respectively. In this case, give a &*step* namelist specifying *ib, ia, k, str* for a coupling from state *ib* to state *ia*, multipolarity *k* and strength *str* (*str* is the reduced matrix element for Coulomb transitions and the reduced deformation length for nuclear transitions).

```
alpha+c12 -> alpha+c12* @ 100 Mev; nuc def
NAMELIST
&FRESCO hcm=0.050 rmatch=20.000 rintp=0.20
        jtmin=0.0 jtmax=40 absend= 0.01
        thmin=0.00 thmax=180.00 thinc=1.00
        iter=1 ips=0.0 iblock=0
        chans=1 smats=2  xstabl=1
        elab(1)=100.0 /

 &PARTITION namep='alpha' massp=4.0000 zp=2
           namet='12C'   masst=12.000 zt=6 qval=0.000 nex=2  /
 &STATES jp=0. bandp=1 ep=0.0000 cpot=1 jt=0.0 bandt=1 et=0.0000 /
 &STATES copyp=1                  cpot=1 jt=2.0 bandt=1 et=4.4390 /
 &partition /

 &POT kp=1 ap=4.000 at=12.000 rc=1.2  /
 &POT kp=1 type=1  p1=40.0 p2=1.2 p3=0.65 p4=10.0 p5=1.2 p6=0.500  /
 &POT kp=1 type=11 p1=0.0  p2=1.3 /
 &POT kp=1 type=2  p1=0.00 p2=1.2 p3=0.65 p4=6.0 p5=1.2 p6=0.500  /
 &POT kp=1 type=11 p1=0.0  p2=1.3 /
 &pot /
 &overlap /
 &coupling /
```

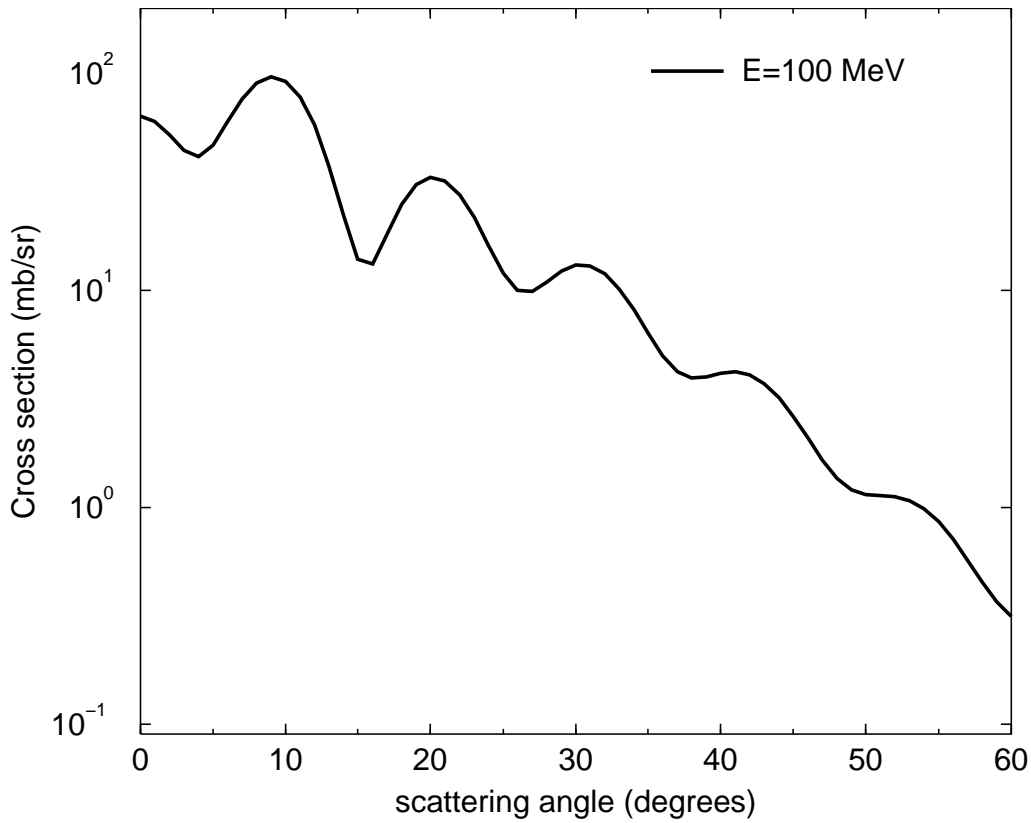Box 2: FRESCO input for the inelastic excitation of ^{12}C by α particles at 100 MeV

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Figure 2: Inelastic angular distribution for the excitation of ^{12}C by α particles at 100 MeV obtained with the input of Box 2.

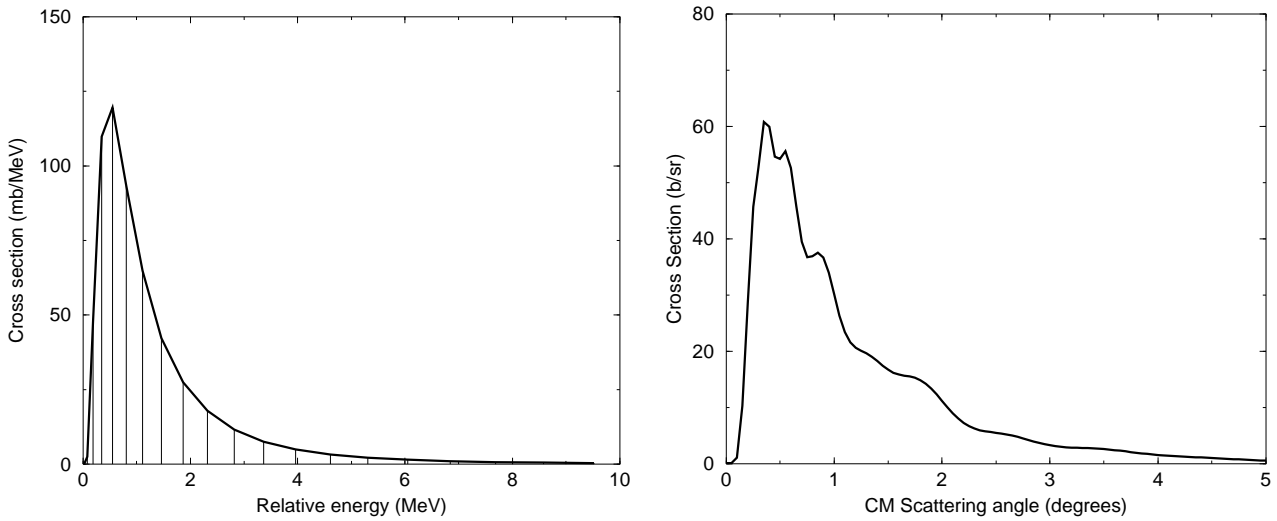Figure 3: Breakup of ^{8}B on ^{208}Pb at 82 MeV/u. Left: p–^{7}Be relative energy distribution. Right: center-of-mass angular distribution. Both are obtained with the input of Box 3.

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```
CDCC 8B+208Pb ; nuclear and coulomb s-wave breakup
NAMELIST
 &Fresco  hcm= 0.01 rmatch= -60.000 rintp=  0.15 rsp=  0.0 rasym=  1000.00 accrcy= 0.001
    jtmin=  0.0 jtmax=  9000.0 absend= -50.0000
    jump =     1     10     50    200
    jbord=    0.0  200.0  300.0  1000.0  9000.0
    thmin=  0.00 thmax=  20.00 thinc=  0.05 cutr=-20.00
    ips= 0.0000  it0= 0 iter=  0 iblock= 21 nnu= 24 smallchan= 1.00E-12  smallcoup= 1.00E-12
    elab=  656.0000    pel=1 exl=1 lab=1 lin=1 lex=1 chans= 1 smats= 2 xstabl= 1 cdcc= 1/
 &Partition namep='8B' massp=  8. zp=  5 nex= 21 pwf=T namet='208Pb' masst=208. zt= 82 qval=  0.1370/
 &States jp= 1.5 ptyp=-1 ep=  0.0000  cpot=  1 jt= 0.0 ptyt= 1 et=  0.0000/
 &States jp= 0.5 ptyp= 1 ep=  0.1583  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  0.2180  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  0.3260  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  0.4830  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  0.6889  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  0.9438  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  1.2478  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  1.6007  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  2.0027  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  2.4536  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  2.9536  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  3.5025  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  4.1005  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  4.7474  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  5.4434  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  6.1884  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  6.9824  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  7.8253  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  8.7173  cpot=  1 copyt= 1/
 &States jp= 0.5 ptyp= 1 ep=  9.6583  cpot=  1 copyt= 1/
 &Partition namep='7Be' massp=  7. zp=  4 nex= -1 pwf=T namet='209Pb' masst=209.0000 zt=83 qval=  0./
 &States jp= 0.0 ptyp= 1 ep=  0.0000  cpot=  2 jt= 0.0 ptyt= 1 et=  0.0000/
 &Partition /
 &Pot kp= 1 type= 0 shape= 0 p(1:3)=   1.0000   0.0000  2.6500 /
 &Pot kp= 2 type= 0 shape= 0 p(1:3)= 208.0000   0.0000  1.3000 /
 &Pot kp= 2 type= 1 shape= 0 p(1:6)= 114.2000   1.2860  0.8530  9.4400  1.7390  0.8090 /
 &Pot kp= 3 type= 0 shape= 0 p(1:3)= 208.0000   0.0000  1.3000 /
 &Pot kp= 3 type= 1 shape= 0 p(1:6)=  34.8190   1.1700  0.7500 15.3400  1.3200  0.6010  /
 &Pot kp= 4 type= 0 shape= 0 p(1:3)=   1.0000   0.0000  2.3910 /
 &Pot kp= 4 type= 1 shape= 0 p(1:3)=  44.6750   2.3910  0.4800 /
 &Pot kp= 4 type= 3 shape= 0 p(1:3)=   4.8980   2.3910  0.4800 /
 &Pot /
 &Overlap kn1=  1 ic1=1 ic2=2 in= 1 kind=0 nn= 1 l=1 sn=0.5 j= 1.5 nam=1 ampl=  1.00 kbpot= 4 be=  0.1370 isc= 1 ipc=0 /
 &Overlap kn1=  2 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -0.0182 isc=12 ipc=2 nk=  20 er= -0.0344 /
 &Overlap kn1=  3 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -0.0771 isc=12 ipc=2 nk=  20 er= -0.0834 /
 &Overlap kn1=  4 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -0.1850 isc=12 ipc=2 nk=  20 er= -0.1324 /
 &Overlap kn1=  5 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -0.3419 isc=12 ipc=2 nk=  20 er= -0.1814 /
 &Overlap kn1=  6 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -0.5479 isc=12 ipc=2 nk=  20 er= -0.2304 /
 &Overlap kn1=  7 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -0.8028 isc=12 ipc=2 nk=  20 er= -0.2794 /
 &Overlap kn1=  8 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -1.1067 isc=12 ipc=2 nk=  20 er= -0.3284 /
 &Overlap kn1=  9 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -1.4596 isc=12 ipc=2 nk=  20 er= -0.3774 /
 &Overlap kn1= 10 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -1.8616 isc=12 ipc=2 nk=  20 er= -0.4264 /
 &Overlap kn1= 11 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -2.3125 isc=12 ipc=2 nk=  20 er= -0.4754 /
 &Overlap kn1= 12 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -2.8125 isc=12 ipc=2 nk=  20 er= -0.5245 /
 &Overlap kn1= 13 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -3.3614 isc=12 ipc=2 nk=  20 er= -0.5735 /
 &Overlap kn1= 14 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -3.9594 isc=12 ipc=2 nk=  20 er= -0.6225 /
 &Overlap kn1= 15 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -4.6064 isc=12 ipc=2 nk=  20 er= -0.6715 /
 &Overlap kn1= 16 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -5.3023 isc=12 ipc=2 nk=  20 er= -0.7205 /
 &Overlap kn1= 17 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -6.0473 isc=12 ipc=2 nk=  20 er= -0.7695 /
 &Overlap kn1= 18 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -6.8413 isc=12 ipc=2 nk=  20 er= -0.8185 /
 &Overlap kn1= 19 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -7.6843 isc=12 ipc=2 nk=  20 er= -0.8675 /
 &Overlap kn1= 20 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -8.5763 isc=12 ipc=2 nk=  20 er= -0.9165 /
 &Overlap kn1= 21 ic1=1 ic2=2 in= 1 kind=0 l=0 sn=0.5 j= 0.5 nam=1 ampl=  1.00 kbpot= 4 be= -9.5173 isc=12 ipc=2 nk=  20 er= -0.9655 /
 &Overlap /  !
 &Coupling icto= 1 icfrom= 2 kind=3 ip1= 2 ip2= 0 ip3= 0 p1=   3.0000 p2= 2.0000 /
 &Coupling /
```

Box 3: FRESCO input for the breakup of ^{8}B on ^{208}Pb at 82 MeV/u

```
8B+208Pb ; N+C breakup with q=0,1,2
CDCC
 &CDCC
  hcm=0.01  rmatch=-60 rasym=1000 accrcy=0.001 absend=-50
  elab=656
  jbord=  0  200 300 1000 9000
  jump =  1  10  50  200
  thmax=20 thinc=0.05 cutr=-20 smats=2 xstabl=1
  ncoul=0 reor=0 q=2
  /
 &NUCLEUS part='Proj' name='8B' charge=5 mass=8
                      spin=1.5 parity=-1 be = 0.137 n=1 l=1 j=1.5 /
 &NUCLEUS part='Core' name='7Be' charge=4 mass=7 /
 &NUCLEUS part='Valence' name='proton' charge=1 mass=1 spin=0.5/
 &NUCLEUS part='Target' name='208Pb' charge=82 mass=208 spin=0 /

 &BIN spin=0.5 parity=+1 start=0.001 step=0.50 end=10. energy=F l=0 j=0.5/
 &BIN /

 &POTENTIAL part='Proj' a1=1 rc=2.65 /
 &POTENTIAL part='Core'    a1=208 rc=1.3 v=114.2 vr0=1.286 a=0.853 w=9.44 wr0=1.739 aw=0.809 /
 &POTENTIAL part='Valence' a1=208 rc=1.3 v=34.819 vr0=1.17 a=0.75 w=15.340 wr0=1.32 aw=0.601/
 &POTENTIAL part='Gs' a1=1 rc=2.391 v=44.675 vr0=2.391 a=.48 vso=4.898 rso0=2.391 aso=0.48 /
```

Box 4: FRESCO input for the breakup of ^{8}B on ^{208}Pb at 82 MeV per nucleon (short version)

namelist *states* needs to be repeated for each bin, with appropriate excitation energy and quantum numbers. Since in this example we are not interested in the second partition, it does not get printed with the option of negative *nex*. Several new variables are needed when defining the bins: negative *be* provides bins with energy relative to threshold $|be|$, with a width *er*, and an amplitude $\sqrt{nam}$*ampl*. To characterize the weight function of the bin we use *isc* (*isc*=2 for non-resonant bins, and *isc*=4 for resonant bins). Note that here, the same potential is used for the ^{8}B bound and continuum states. This need not be the case.

After defining the overlaps, coupling parameters are introduced: *kind=3* stands for single-particle excitations of the projectile (*kind=4* would be for the target), *ip1* is the maximum multipole order in the expansion of the couplings included, *ip2*=0,1,2 for Coulomb and nuclear, nuclear only and Coulomb only, respectively, and *ip3* makes specific selections of couplings with default *ip3*=0 when all couplings are included.[9] For the interactions in the coupling matrix, the core-target is potential index *p1*=3 and the valence-target is potential index *p2*=2.

Angular distributions of the cross sections for each energy bin can be found in fort.16. To obtain a total angular distribution one needs to sum over all bins (use sumbins < fort.16 > xxx.xsum). For the breakup example shown here, the resulting total angular distribution is plotted in Fig. 3(left). If you are interested in the energy distribution, fort.13 contains all angular integrated cross sections for each bin. In general, for each energy, a sum over all ℓ partial waves within the projectile is necessary (use sumxen < fort.13 > xxx.xen). In Fig. 3(right) we show the energy distribution for the ^{8}B breakup here considered. In addition, it is useful to look at fort.56 (cross section per partial wave *L*) to ensure that enough partial waves are included in the calculation. Defining a long list of bin states and overlaps can be easily automated. The revised CDCC style of input has been developed specifically for large CDCC calculations, and transforms a simpler input into the standard input we have just gone through. The simpler input would then look like Box 4.

---

[9]If *ip3*=1, there are no reorientation couplings for all but the monopole, if *ip3*=2, only reorientation couplings are included, and if *ip3*=3 it includes only couplings to and from the ground state. More options exist but are not presented here.

```
n14(f17,ne18)c13 @ 170 MeV;
NAMELIST
 &FRESCO hcm=0.03 rmatch=40 rintp=0.20 hnl=0.1 rnl=5.00 centre=0.0
            jtmin=0.0  jtmax=120 absend=-1.0
            thmin=0.00 thmax=40.00 thinc=1.00
            iter=1 nnu=36
            chans=1 xstabl=1
            elab=170.0  /

 &PARTITION namep='f17'  massp=17. zp=9 namet='n14'  masst=14. zt=7 nex=1  /
 &STATES jp=2.5 bandp=1 ep=0.0 cpot=1 jt=1.0 bandt=1 et=0.0000  /

 &PARTITION namep='ne18' massp=18. zp=10 namet='c13'  masst=13. zt=6 qval=3.6286 nex=1  /
 &STATES jp=0. bandp=1 ep=0.0  cpot=2 jt=0.5 bandt=-1 et=0.0000  /
 &partition /

 &POT kp=1 ap=17.000 at=14.000 rc=1.3  /
 &POT kp=1 type=1 p1=37.2 p2=1.2 p3=0.6  p4=21.6 p5=1.2 p6=0.69  /
 &POT kp=2 ap=18.000 at=13.000 rc=1.3  /
 &POT kp=2 type=1 p1=37.2 p2=1.2 p3=0.6  p4=21.6 p5=1.2 p6=0.69  /
 &POT kp=3 at=17 rc=1.2  /
 &POT kp=3 type=1 p1=50.00 p2=1.2 p3=0.65   /
 &POT kp=3 type=3 p1=6.00  p2=1.2 p3=0.65   /
 &POT kp=4 at=13 rc=1.2  /
 &POT kp=4 type=1 p1=50.00 p2=1.2 p3=0.65   /
 &POT kp=4 type=3 p1=6.00  p2=1.2 p3=0.65   /
 &POT kp=5 ap=17.000 at=13.000 rc=1.3  /
 &POT kp=5 type=1 p1=37.2 p2=1.2 p3=0.6  p4=21.6 p5=1.2 p6=0.69  /
 &pot /

 &Overlap kn1=1 ic1=1 ic2=2 in=1 kind=0 nn=1 l=2 sn=0.5 j=2.5 kbpot=3 be=3.922  isc=1 ipc=0 /
 &Overlap kn1=2 ic1=2 ic2=1 in=2 kind=3 nn=1 l=1 sn=0.5 ia=1 ib=1 j=1.0 kbpot=4 be=7.5506 isc=1 ipc=0 /
 &overlap /

 &coupling icto=-2 icfrom=1 kind=7 ip1=0 ip2=-1 ip3=5 /
 &CFP in=1 ib=1 ia=1 kn=1 a=1.00  /
 &CFP in=2 ib=1 ia=1 kn=2 a=1.00  /
 &CFP /
 &coupling /
```

Box 5: FRESCO input for the transfer reaction ^{14}N(^{17}F,^{18}Ne)^{13}C at 10 MeV/u.

2.4 Transfer

Transfer reactions are often used to extract structure information to input in astrophysical simulations. Here we consider the ^{14}N(^{17}F,^{18}Ne)^{13}C transfer reaction at 10 MeV per nucleon. This reaction was measured with the aim of extracting the asymptotic normalization coefficient of specific states in ^{18}Ne which in turn provides a significant part of the rate for ^{17}F(p,γ). The proton capture reaction on ^{17}F appears in the *rp*-process in novae environments. The ratio of the proton capture rate and the decay rate of ^{17}F is also very important for the understanding of galactic ^{17}O, ^{18}O and ^{15}N. The input for the transfer example is given in Box 5.

A few important new parameters need to be defined when performing the transfer calculation. Because the process involves a non-local kernel $V^o_{fi}(R',R)$, in addition to the radial grids already understood, we need to introduce *rintp, hnl, rnl, centre*. The *rintp* is the step in R, *hnl, rnl* are the non-local step and the non-local range in $R' - R$, respectively, and centered at *centre*. Gaussian quadrature is used for the angular integrations in constructing the non-local kernels, and *nnu* is the number of the Gaussian integration points to be included.

In this example the core has non-zero spin, and in order to generate the appropriate overlap of the composite nucleus ^{14}N, it is necessary to take into account, not only the angular momentum of the neutron but also the spin of ^{13}C. This can be done with *kind*=3 in the overlap definition where the spin of the core *ia* and of the composite *ib* need to be specified. The coupling scheme is $|(l_n,s_n)j,I_A;I_B\rangle$.

The only other new part of the input concerns the transfer coupling itself, as all other parts (partitions, potentials and overlaps) have already been previously presented. Transfer couplings are defined in the namelist &*cou-*
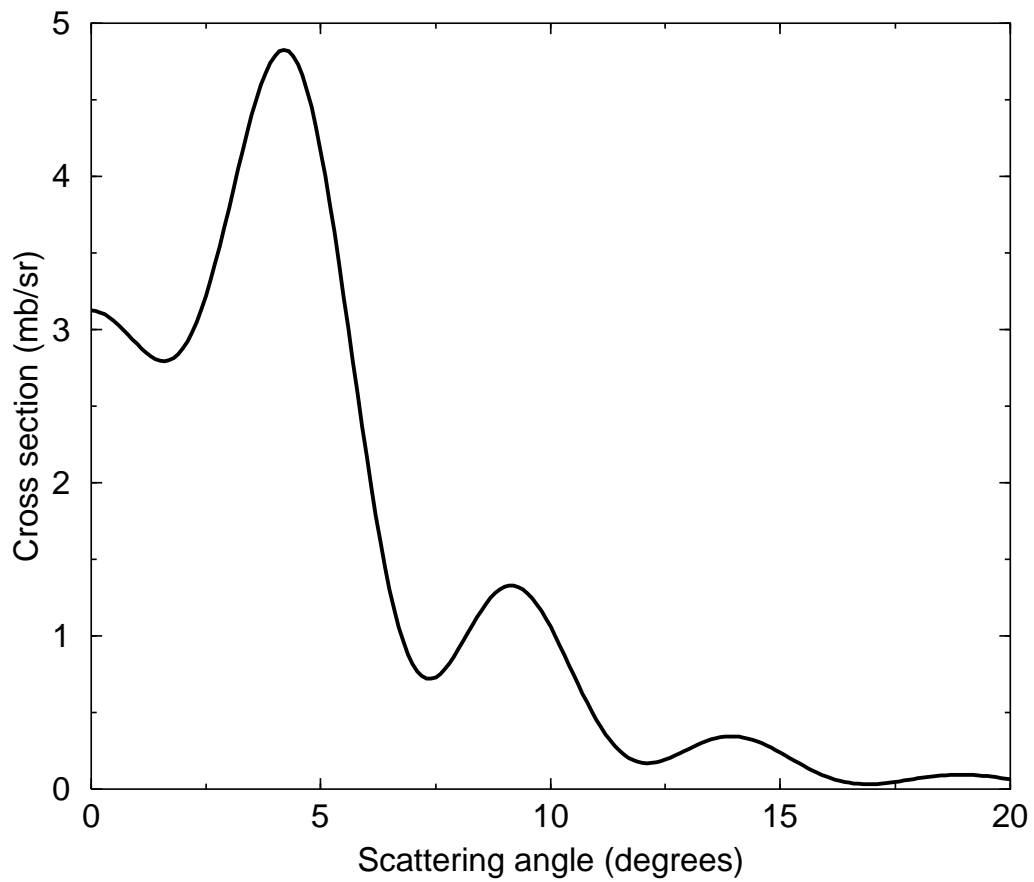
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Figure 4: Transfer cross section for ^{14}N(^{17}F,^{18}Ne)^{13}C at 10 MeV/u calculated with the input of Box 5.

```
14C(n,g)15C E1 only
NAMELIST
 &FRESCO hcm= 0.100 rmatch=100
      jtmin=0 jtmax=4.5 absend=-1
      thmin=0 thmax=0 iter=1
      elab(1)= 0.005 4.005 nlab=50/

 &PARTITION namep='neutron' massp=1.0087 zp=0 nex=1 namet='14C' masst=14.0032 zt=6 /
 &STATES jp=0.5 ptyp=1 ep=0 cpot=1 jt=0.0 ptyt=1 et=0/

 &PARTITION namep='Gamma' massp=0 zp=0 nex=1 namet='15C' masst=15.0106 zt=6 qval=1.218 /
 &STATES jp=1.0 ptyp=1 ep= 0 cpot=3 jt=0.5 ptyt=1 et=0/
 &partition /

 &Pot kp=1 type= 0 shape= 0 p(1:3)=  14.0000   0.0000   1.3000 /
 &Pot kp=1 type= 1 shape= 0 p(1:3)=  57.0000   1.7   0.7000 /
 &Pot kp=1 type= 3 shape= 0 p(1:3)=   0.0000   1.7   0.5000 /
 &Pot kp=2 type= 0 shape= 0 p(1:3)=  14.0000   0.0000   1.2000 /
 &Pot kp=2 type= 1 shape= 0 p(1:3)=  55.7700   1.2230   0.5000 /
 &Pot kp=2 type= 3 shape= 0 p(1:3)=   5.0000   1.2230   0.5000 /
 &pot /

 &OVERLAP kn1=1 ic1=1 ic2=2 in=-2 kind=0 nn=2 l=0 sn=0.5 j=0.5 kbpot=2 be=1.218 isc=1 /
 &overlap /

 &COUPLING icto=2 icfrom=1 kind=2 ip1=-1 ip2= 1/
 &cfp  in=2 ib=1 ia=1 kn=1  a=1.000    /
```

Box 6: FRESCO input for neutron capture by ^{14}C.

pling by *kind*=5,6,7 for zero-range, low energy approximation and finite range, respectively. For finite-range transfers, *ip1*=0,1 stands for post or prior, *ip2*=0,1,−1 for no remnant, full real remnant and full complex remnant respectively and *ip3* denotes the index of the core-core optical potential. If *ip3*=0 then it uses the optical potential for the first pair of excited states in the partition of the projectile core.

Following the &*coupling* namelist, we need to define the amplitudes (coefficients of fractional parentage) of all the overlaps to be included in the calculation. Here, this is done with &*cfp* where *in*=1,2 for projectile or target, *ib/ia* corresponds to the state index of the composite/core and *kn* is the index of the corresponding overlap function. So the first &*cfp* refers to the $\langle^{17}\text{F}|^{18}\text{Ne}\rangle$ overlap and the second &*cfp* refers to the $\langle^{13}\text{C}|^{14}\text{N}\rangle$ overlap. The angular distribution obtained from our example is presented in Fig. 4.

2.5 Capture

Capture reactions are of direct interest in astrophysics. Although the electromagnetic operator is well understood, coupling effects may be non-trivial and require focused work. Here we pick a neutron capture reaction that is completely dominated by $E1$: $^{14}\text{C}(n,\gamma)^{15}\text{C}$. This reaction was first introduced in the context of the *r*-process. In our example, the capture is calculated at 50 different scattering energies, from 5 keV up to 4 MeV. The input is presented in Box 6

For capture reactions, the first partition is defined in the usual way, but in the second partition, the projectile should be *Gamma* (with spin *jp*=1 and positive parity) and *cpot* should refer to a non-existing potential in order that there be no photon potential. The $2s_{1/2}$ ^{15}C overlap is defined in &*overlap*. Electromagnetic one-photon couplings are defined through *kind*=2. Therein, *ip1* refers to the multipolarity of the transition and *ip2*=0,1,2 for including both electric and magnetic transitions, electric only and magnetic only, respectively. If *ip1* > 0, all multipolarities up to *ip1* are included, otherwise only |*ip1*| is calculated.

There are several outputs available specifically for astrophysics. In Fig. 5 we plot the cross section for the $^{14}\text{C}(n,\gamma)^{15}\text{C}$ capture reaction as a function of center-of-mass energy (found in fort.39). For charged-particle

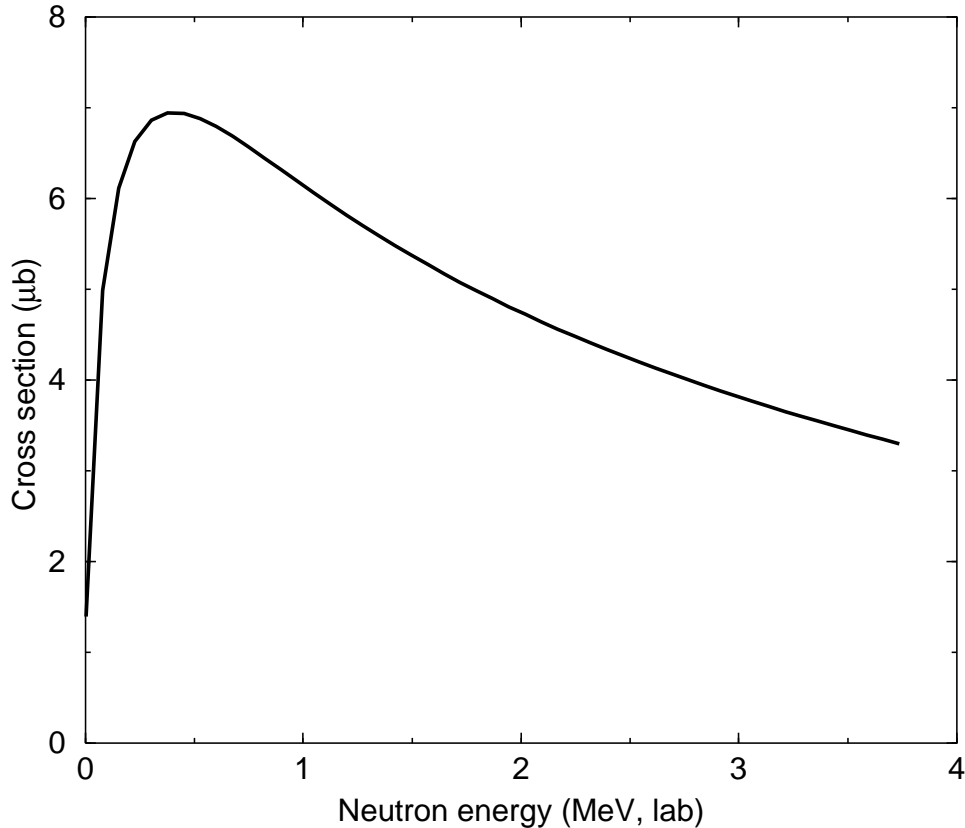Figure 5: Neutron capture cross section for ^{14}C as a function of neutron energy and calculated with the input of Box 6.

reactions, astrophysical S-factors are also available (see Table 1).

3 Runtime errors

In a complicated modeling computer program like FRESCO, accurate results cannot be obtained if there are obvious numerical errors either in the input, or produced during the calculation. Problems may occur at energies very much below the Coulomb barrier, or at relativistic energies, since FRESCO should not be used in these cases. The program is written to stop when large numerical inaccuracies occur, but no results can be trusted until they are examined to see that they are not sensitive to further increases to the maximum radius *rmatch*, maximum partial waves *jtmax*, maximum non-local range *rnl*, and further decreases in the radial step size *hcm* and lower radial cutoff parameter *cutl*. We give some guidance on these parameters below.

When the program reads the input file, typing errors in variables or their values will cause the program to stop after printing out the complete namelist so you can see which variables have been successfully read in. Alternatively, if the words NAMELIST and CDCC in the second line of the input are written in lower case ('namelist' or 'cdcc'), the compiler's own error handling will be used instead. You can also look at the input echo in fort.3, to see up to which line the input has been read successfully.

During the running of FRESCO, a number of induced or cancellation errors can be detected. These are:

Step size too large: If k is the asymptotic wave number for a channel, then its product with the step size should be sufficiently small for the Numerov integration method to avoid large errors: $k * hcm < 0.2$.

Bound-state search failure: Bound states are found in subroutine eigcc by a Newton-Raphson method with at most 40 iterations. Such states can be found at a specific energy by varying some part of the potential: this part cannot be zero.

Insufficient non-local width: If the non-local coupling form factors are too large when $|R - R'| \geq rnl$, then *rnl* should be increased as recommended.

L-transfer accuracy loss: In the transfer Legendre expansion, if $\ell + \ell'$ is too large, there can be cancellation errors between different multipoles T. This can be remedied by increasing the input parameter *mtmin* to use the slower *m*-dependent method of [1].

Matching deficiency: The program will print an error message if the nuclear potentials are not smaller than 0.02 MeV at the outer matching radius, and stop if they are larger than 0.1 MeV. Increase *rmatch*, or correct some potential that does not decay sufficiently fast.

Iteration failure in solving coupled equations: If in some partial wave set, more than *iter* iterations still do not appear to converge, then all cross sections will be affected. Either use Padé acceleration, increase *iter* or make it negative so that the 'best' intermediate value is used, or increase *ips* slightly. The detailed progress of the iterations can be seen by setting $smats \geq 5$.

Accuracy loss in solving coupled equations: If any of the channels are propagating in a classically forbidden region, there will be loss of linear independence of the separate solutions $\{Y_{\alpha\beta}(R)\}$, as all solutions will tend to become exponentially increasing. This is monitored in the subroutine erwin during the summations, and will lead to a halt if the cancellation errors are expected to be more than 3%. In this case, increase the lower cutoff parameters *cutl* or *cutr*, decrease the matching radius *rmatch* if possible, or else use the R-matrix expansion method to solve the equations. An extreme error occurs if the simultaneous equations from the matching conditions are singular.

Internal parameter error: Sometimes, the precalculation of array sizes is inadequate. For advanced users these can be improved by selective specification of the maxcoup(1:3) and expand(1:11) input arrays.

At the end of a FRESCO calculation, a final 'accuracy analysis' is presented. This rechecks that the step size *hcm* is small enough, and that *rnl* is large enough. Then, using the Coulomb trajectories, it calculates the minimum scattering angles expected to be accurate because of the finite values of *rmatch* and *jtmax*.

4   Fitting data: SFRESCO

A first calculation of cross sections using FRESCO will rarely be near the experimental data. Perhaps the reaction model is too simplified, or perhaps the input parameters are not accurate enough. The optical potential, binding potentials, spectroscopic amplitudes or R-matrix reduced widths could well be adjusted to see if the agreement between theory and experiment can be improved. The program SFRESCO searches for a χ^2 minimum when comparing the outputs of FRESCO with sets of data, using the MINUIT search routines.

The inputs for SFRESCO specify the FRESCO input and output files, the number and types of search variables, and the experimental data sets to be compared with. These experimental data can be (*type*=0) an angular distribution for fixed energy, (1) an excitation and angular cross-section double distributions, or (2) an excitation cross section for fixed angle. They could also be (3) an excitation function for the total, reaction, fusion or inelastic cross section, (4) an excitation phase shift for fixed partial wave, (5) a desired factor for bound-state search, or (6) even a specific experimental constraint on some search parameter.

The simplest and most common fitting requirement is to determine an optical potential to fit the observed elastic scattering angular distribution. For example, to find a proton optical potential to fit cross sections for scattering on ^{112}Cd at 27.90 MeV, we start with the normal FRESCO input of Box 7. The cross sections will be calculated at the experimental angles, not those specified here. In order to vary the real and imaginary potential strengths in this input, as well as the real radius, we have the search file for SFRESCO of Box 8. This search file begins

```
p + 112Cd elastic
NAMELIST
 &FRESCO  hcm= 0.100 rmatch=  20.000 jtmin=  0.0 jtmax=  200.0
    thmin=  0.00 thmax=180.00 thinc=  2.00 xstabl= 1
    elab(1)=   27.9 /
 &PARTITION namep='Proton ' massp=  1.0000 zp=  1 nex= 1
        namet='112Cd   ' masst=112.0000 zt= 48 qval=  0/
 &STATES jp= 0.5 ptyp= 1 ep=  0.0000  cpot=  1 jt= 0.0 ptyt= 1 et=  0.0000/
 &partition /
 &pot kp= 1 type= 0 p(1:3)=  112.000  0.0000  1.2000 /
 &pot kp= 1 type= 1 p(1:6)=   52.500  1.1700  0.7500  3.5000  1.3200  0.6100  /
 &pot kp= 1 type= 2 p(1:6)=    0.000  0.0000  0.0000  8.5000  1.3200  0.6100  /
 &pot kp= 1 type= 3 p(1:3)=    6.200  1.0100  0.7500 /
 &pot /
 &overlap /
 &coupling /
```

Box 7: FRESCO input file p-cd.frin for proton scattering on ^{112}Cd

```
'p-cd.frin' 'p-cd.frout'
4 1
 &variable kind=1 name='r0' kp=1 pline=2 col=2 potential=1. step=0.01/
 &variable kind=1 name='V' kp=1 pline=2 col=1 potential=50.0 step=0.1/
 &variable kind=1 name='W' kp=1 pline=2 col=4 potential=5.0 step=0.1/
 &variable kind=1 name='WD' kp=1 pline=3 col=4 potential=10. step=0.1/
 &data iscale=0  idir=1 lab=F abserr=T/
 22.     0.548    0.044
 26.     0.475    0.024
 30.     0.481    0.014
 38.     0.447    0.009
 50.     0.144    0.004
 66.     0.499    0.010
 70.     0.248    0.005
 86.     0.463    0.014
 90.     0.485    0.015
 106.    0.087    0.003
 110.    0.135    0.004
 130.    0.161    0.005
 &
```

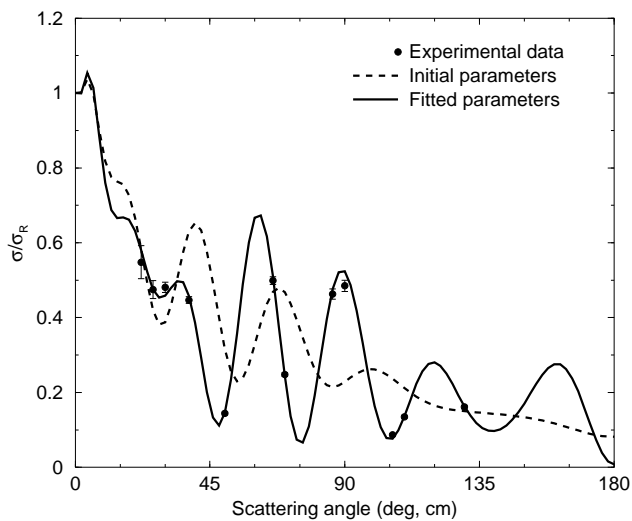Box 8: SFRESCO input p-cd.search for proton scattering on ^{112}Cd

Figure 6: Initial and fitted proton scattering on ^{112}Cd at 27.9 MeV.

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Table 2: SFRESCO input commands. Words in `typewriter font` are to be replaced with user values.

Command	Operation
Q	query status of search variables
SET `var val`	set variable number `var` to value `val`.
FIX `var`	fix variable number `var` (set `step=0`).
STEP `var step`	unfix variable `var` with step `step`.
SCAN `var val1 val2 step`	scan variable `var` from value `val1` to `val2` in steps of `step`.
SHOW	list all datasets with current predictions and χ values.
LINE `plotfile`	write file (default: **search.plot**) with theoretical curves only.
READ `file`	read plot output `file` for further searches, if not:
READ `snapfile`	if the name of `snapfile` contains the string 'snap',
	read last set of snap output `snapfile` from a previous fort.105.
ESCAN `emin emax estep`	scan lab. energy in incident channel
MIN	call MINUIT interactively.
MIGRAD	in MINUIT, perform MIGRAD search.
END	return to SFRESCO from MINUIT.
PLOT `plotfile`	write file (default: **search.plot**) with data and theory curves.
EX	exit (also at end of input file)

by identifying the previous FRESCO input and naming the temporary output file, then giving the number of search variables and the number of experimental data sets.

There are 3 *&pot* namelist lines in Box 7 for the nuclear parts of potential *kp*=1, so the variables of the interaction potentials (*kind*=1) in the search are identified by the specification of *kp* and *pline* in the *&variable* namelist in Box 8, along with *col* for the index to the *p* array. The *potential* value gives the initial value for the search, and *step* the initial magnitude for trial changes. Deformations can as well be searched upon. There are also parameters *valmin* and *valmax*,[10] to limit the range of that variable. Spectroscopic amplitudes to be varied (*kind*=2) are identified by the order *nfrac* in which they appear in the FRESCO input in a *&cfp* namelist, and then by their initial value *afrac*. Other variable *kind*s are described in the FRESCO input manual.

Experimental data sets are identified by their *type* specifications as listed above, and then by *data_file* for name of data file with data, which can be '=' for this search file, '<' for stdin (the default is '='). Then *points* gives the number of data points (default: keep reading as many as possible), *lab* is T or F for laboratory angles and cross sections (default false), and *energy* is lab energy for a *type*=0 dataset (default: use *elab(1)* from *&fresco* namelist). The *abserr* is true for absolute errors (default: false). Next, *idir* is −1 for cross-section data given as astrophysical S-factors, 0 for data given in absolute units (the default), and 1 as ratio to Rutherford. Finally, *iscale* is −1 for dimensionless data, and 0 absolute data in units of fm^2/sr, 1 for b/sr, 2 for mb/sr (the default) and 3 for μb/sr.

With these two files (Boxes 7 and 8), SFRESCO is invoked interactively. First the name of the search file in Box 8 is given, then commands as in Table 2. A minimum set of commands will be **p-cd.search** / **min** / **migrad** / **end** / **plot**. The output plot file (default name **search.plot**) also contains the final values of the searched variables. The fitted parameters in this example are $V = 52.53$ MeV, $r0 = 1.179$ fm, $W = 3.46$ MeV and *WD* = 7.43 MeV with $\mathcal{X}^2/N = 2.19$. The initial and final fits to the data are shown in Fig. 6.

5   System requirements, compilations and installation

The website **www.fresco.org.uk** contains a complete distribution set of files for FRESCO and SFRESCO, SUMBINS and SUMXEN. It contains the input and output files for all the examples described here. The distribution files also contain input and output files for a range of test cases for your installation, as well as copies

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[10]Both or none of these must be present.

of the detailed input manuals for FRESCO and MINUIT.

The distribution set contains a set of precompiled binaries for FRESCO and SFRESCO, as well as the source code. To compile the source, you will need a FORTRAN compiler for at least Fortran 90 or 95. The code is in the directory fres/source/, where the script mk attempts to find the best compiler for your system, and then compile in a subdirectory named by your system architecture *arch* and the compiler chosen using the makefile. You may have to edit the makefile to set FFLAGS for your compiler, and set TIME and FLUSH according to your system libraries. After compilation, mk install copies the binaries to a standard bin/*arch*/ directory for execution in other places.

The website will be regularly updated to include descriptions of any further changes needed or advisable for the programs. All of the information on the website is published under the conditions of the GNU Public License described at www.gnu.org/copyleft/gpl.html.

References

[1] T. Tamura, T. Udagawa, K. E. Wood and H. Amakawa, *Comput. Phys. Commun.* **18** (1979) 63.