

# Fresco

I.J. Thompson

Nuclear Theory and Modelling, Livermore National Laboratory, Livermore CA 94551, USA  
and

Department of Physics, University of Surrey, Guildford GU2 7XH, England.

Email: I-Thompson@llnl.gov or Ian@kernz.org

Version FRES 3.2, November 2017  
LLNL-SM-485670

## 1 Introduction

FRESCO is a Coupled-Channels program that can have finite-range transfer interactions among any number of mass partitions, and any number of nuclear excitations in each partition.

This is accomplished by calculating and storing the kernels of the non-local interactions, and then solving the coupled-channels set iteratively. At each iteration the stored kernels are used to integrate the wave functions to generate the source terms for the next iteration. Pade approximants can be used if the iterations diverge because of strong couplings.

The program can also generate local couplings for the rotational or single-particle excitations of either the projectile or the target in any partition, the local form factors for zero-range or local-energy-approximation can also be used. These various local interactions may also be included iteratively (to give multistep DWBA), or alternatively the first few coupled channels may be blocked together and solved by exact coupled-channels methods.

Special treatment is provided for any long ranged Coulomb multipoles, using James Christley's coupled-Coulomb functions CRCWFN, and interpolation in partial waves is also possible.

The nonlocal kernels for single-particle transfers are calculated first at a much smaller number of interpolation points, and then expanded when necessary to calculate the source terms by integrating

$$S(R_f) = \int_0^{R_{match}} K_{fi}(R_f, R_i) u(R_i) dR_i$$

where RMATCH and HCM, the step size, are given on card 1. Since the kernel function  $K_{fi}(R_f, R_i)$  is usually rapidly varying with  $D_{fi} = R_f - R_i$  (especially with heavy-ion reactions), and only slowly varying with  $R_f$  (if  $D_{fi}$  is constant), FRESCO calculates and stores the function  $K'_{fi}(R_f, D_{fi})$  at intervals of RINTP (card 1) in  $R_f$ , and intervals of HNL in  $D_{fi}$ . The  $D_{fi}$  range considered is CENTRE-RNL/2 to CENTRE+RNL/2, i.e. range of RNL centred at CENTRE, and FRESCO later suggests improved values for RNL & CENTRE. The HNL reflects to physical variation of  $K'_{fi}$  with  $D_{fi}$ , and can be a fraction of HCM (for heavy ion reactions) or a multiple of HCM (for light ion reactions)

especially with ‘prior’ interactions). If HNL is a submultiple of HCM, the program anticipates the interpolation of  $u(R_i)$  in the equation above, and only stores an effective kernel function at intervals of HCM.

The new variable MTMIN in the FRT version controls the method used to calculate the form factors of the transfer kernels. If the L-transfer value (estimated by  $\ell_f + \ell_i$ ) is larger than or equal to MTMIN, then the m-dependent expressions for the spherical harmonics are used explicitly. Otherwise, the angular dependencies of the initial and final transfer states are transformed into those of the channel variables  $R_i$  &  $R_f$  using Moshinsky’s solid-harmonic transformation, as given for example in Austern et al. Phys. Rev. **133** pp B 3 - 16. By careful control of the numerical approximations, the second method can be extended to find heavy-ion transfer form factors, but the maximum transferred angular momentum L is still limited by numerical cancellation errors arising from the finite roundoff errors in the computer. With 8-byte word lengths, the unit roundoff is approximately  $10^{-15}$ , and this limits the transferred L to 6 or less, so the default value of MTMIN is set to 6. The Moshinsky method is much faster when it is accurate, so the default value of MTMIN has been set as high as practical.

A general description of the formalisms used is given in I.J. Thompson, *Coupled Reaction Channels Calculations in Nuclear Physics*, Computer Physics Reports, **7** (1988) pp 167 - 212.

## 2 Input Cards

### 2.1 Definition Cards

#### Card 0

10A8 HEADNG(10)

Heading to describe the nature of this run, for user's information only.

#### Card 1

10F8.4 HCM, RMATCH, RINTP, HNL, RNL, CENTRE

Wave functions calculated at intervals of HCM up to abs(RMATCH).

If RMATCH < 0, then read Card 1a for coupled Coulomb wave functions.

Non-local kernels  $K'_{fi}(R_f, D_{fi})$  calculated at  $R_f$  intervals of RINTP, and for a non-local ( $D_{fi}$ ) range of RNL centred at CENTRE in steps of HNL. RMATCH and RINTP are rounded to multiples of HCM, and HNL is rounded either to a multiple or a sub-multiple of HCM.

#### Card 1a

2F8.6, 2F8.2 RASYM, ACCUR, SWITCH, AJSWITCH

Use coupled Coulomb wave functions from CRCWFN out to asymptotic radius RASYM from inner radius abs(RMATCH) for those partitions in which PWF is TRUE.

If RASYM < 0, then determine the outer radius in order that classical Coulomb trajectories reach an angle abs(RASYM) degrees.

ACCUR is an accuracy parameter controlling the piecewise step length. Default is 0.01: smaller values give greater accuracy.

SWITCH is the radius at which to switch from Airy functions to sines and cosines in piecewise method. Default is 1000 fm.

AJSWITCH - default is 0.0

Normally the Coupled Coulomb wfns are matched to zero and the Numerov integration is omitted, when the Coulomb distance of closest approach is more than 4.5 fm outside abs(RMATCH) (or the -CUTR distance if CUTR negative). This is only allowed when  $J_{total} \geq \text{AJSWITCH}$ .

#### Card 2

2F4.0, F8.4, L2, I2, 1X, A1, I2 4(I4, F4.0)  
JTMIN, JTMAX, ABSEND, DRY, CSET, RELA, NEARFA, (JUMP(i), JBORD(i), i=2, 5)

Calculate coupled-channels sets with total J in the interval  $\max(0, \text{JTMIN}) < J < \text{JTMAX}$ , stopping sooner if the absorption from the elastic channel is less than ABSEND millibarns of three successive J/parity sets. (If ABSEND < 0, this takes the full J interval.)

If JTMIN < 0, then for  $J < \text{abs}(\text{JTMIN})$  include only the incoming channel in the calculations, ignoring transfers and excited states. This is needed if the elastic scattering cross sections are to be given correctly.

DRY is normally F (false), but if T (true) the code does a 'dry run' to check that all arrays are of sufficient size.

All coupled channel sets are generated, but only the elastic channels should be non-zero.

CSET = number of coupled-channels sets to be solved, for each energy on Card 19. CSET = 0, blank or F, for no special limit.

If CSET = 'P', include only positive parity coupled channels sets,

If CSET = 'M' or 'N', include only negative parity coupled channels sets.

RELA = 'T' for relativistic kinematics for the incident projectile. *Not yet implemented.*

NEARFA

= 0 or 1 for the usual cross sections,

= 2 or -2 for printing 'far side' cross sections too,

= 3 or -3 for printing far and near side cross sections too.

> 0 for printing far & near-sides for elastic channel only.

< 0 for printing far & near-sides for all channels.

JUMP(i),JBORD(i) : Calculate coupled-channels sets not for every J value, but at intervals of JUMP(i) for  $J \geq \text{JBORD}(i)$ , for  $i=1,5$ . (The program sets JUMP(1)=1 & JBORD(1)=JTMIN, to give no J jumping initially). The omitted J values are provided by interpolation on the scattering amplitudes  $A(m'M' : mM; L)$  prior to calculating cross sections.

### Card 3

2I1,F6.4,F8.4,F8.4,I1,3F8.4,I2

KQMAX,PP,THMIN,THMAX,THINC,KOORDS,CUTL,CUTR,CUTC,DGAM

Give cross sections (and tensor analysing powers up to rank  $K = KQMAX$ ) for centre-of-mass scattering angle from THMIN to abs(THMAX) in steps of THINC.

Elastic channels normally output the ratio to Rutherford, unless THMAX < 0.

Calculate analysing powers/polarisations for projectile (PP=0 or blank), target (PP=1), ejectile (PP=2) or residual nucleus (PP=3). PP=4 gives projectile (PP=0) analysing powers, along with Kyy results.

If DGAM>0: generate angular distributions for gammas of lowest allowed multiplicity for decay of excited states of whichever final nucleus is specified by PP (2 or 3), using Legendre polynomials of orders  $\leq KQMAX$ . Distributions are given for 100% decays to all states lower in energy, using smallest allowed multipoles.

KOORDS determines the coordinate systems used for the analysing powers:

KOORDS

= 0 : Madison coordinates (default)

= 1 : Madison + Transverse

= 2 : Madison + Transverse + Recoil

= 3 : Madison + Transverse + Recoil + Hooton-Johnson

CUTL = radial points per L (angular momentum of partial wave) of lower radial cutoff when integrating the radial equations. Default = -1.6

When CUTL>0, use  $\ell = J_{total}$  (total angular momentum of CC set),

When CUTL<0, use  $\ell = L_{in}$  (orbital angular momentum of incoming partial wave).

Using CUTL<0 gives more accurate analysing powers.

CUTR = lower radial cutoff (fm). Use max(CUTL\* $\ell$ \*HCM,CUTR).

If CUTR < 0, put cutoff at point-Coulomb turning point  $-|CUTR|$ .

CUTC = lower radial cutoff (in fm) for off-diagonal couplings.

#### Card 4

F6.4, I2, I4, I2, I2, A1, I3, 2I4 I2, F6.4  
IPS, IT0, ITER, IBLOCK, PADE, ISO, NNU, MAXL, MINL, MTMIN, EPC,

2F8.4 2I2, 2e8.1, 4x, i4  
ERANGE, DK, INH, plane, smallchan, smallcoup, initwf

Solve the coupled channels equations by at least IT0 iterations, and up to ITER iterations. Stop sooner if the absolute differences between successive S-matrix elements (scaled by  $(2J+1)/(2.JTMAX+1)$ ) are less than IPS percent. (Excited state pairs with IGNORE set on Card 7 are not counted against IPS).

Putting IT0=ITER zero solves only the elastic channel (along with the IBLOCK channels: see below). Putting IT0=ITER = 1 or 2 etc. gives 1 or 2-step DWBA.

Normally, a run is terminated if more than ITER steps are required for convergence. Setting ITER < 0 allows continuation even after convergence has failed after abs(ITER) iterations.

Iterations are normally also stopped if the successive differences are smaller than the errors estimated for the numerical integration of the coupled equations. Setting IPS < 0 uses abs(IPS), without this extra check.

IBLOCK is the number of pairs of excitation levels (starting from partition 1, excitation 1) that are coupled exactly by blocking together.

If IBLOCK < 1, then read Card 4.5 (see below) for R-matrix solution of the coupled equations.

PADE

= 0 for no Pade acceleration,

= 1 for Pade acceleration by the epsilon algorithm.

ISO (not implemented in this version)

NNU is the number of Gaussian integration points in the angular integration used for the non-local transfer kernels. NNU should be a multiple of 6; NNU = 18 is the minimum, and 24 or 36 give acceptable accuracy for all the reactions tried so far.

MAXL, MINL are the maximum and minimum L values for the non-local kernels. If zero, MAXL has the default value JTMAX+6, and if MINL < 0 it takes the default value |JTMIN|-6.

MTMIN is the lowest L-transfer for calculating transfer form factors using the m-dependent expressions for spherical harmonics. Putting MTMIN = 0 gives default value MTMIN = 6 (use MTMIN < 0 to avoid invoking default, if all transfers are to use this method).

EPC = percentage cutoff accuracy in the NNU angular integration. If zero, the default is  $(30/NNU)^2\%$ .

ERANGE, DK – *ignored*

INH

= 0 : zero-range transfer forms in intervals of HCM exactly

= 1 : stored in steps of HCM \* (proj. core)/(proj. composite mass)

= 2 : stored in steps of HCM \* (targ. core)/(targ. composite mass)

So INH=2 corrects for longitudinal recoil during transfers with zero-range projectiles.

PLANE = 1,3: zero Coulomb potential for elastic channel

= 2,3: zero Coulomb potentials for all nonelastic channels.

SMALLCHAN = fraction of unitarity to define a 'small channel'.

A channel that is 'small' for NSMALL=2 times is dropped permanently.

SMALLCOUP = if all nonelastic channels are weaker than the fraction SMALLCOUP of unitarity, then permanently change from coupled-channels to DWBA.

INITWF = file number from which to read fixed channel wave functions during all iterations. The channels whose wfs are changed must have the same IT index, that counts cards 7 as excited state pairs. This file

as the same format as the fort.17 produced when WDISK is nonzero. The INITWF > 0 for formatted wf file, and < 0 for unformatted (the same sign convention as for WDISK).

#### Card 4.5

If IBLOCK<0, then read:

```
2i4,          I1,      L1,      I2,  i2,      f6.4, 3f8.4,
NRBASES, NRBMIN, BUTTLE, PRALPHA, PCON, MEIGS, RMATR, EBETA(2), WEAK
```

NRBASES = target number of radial basis states in each channel. (Use 2\*NRBASES for the elastic and first-inelastic channel for more accuracy).

NRBMIN = minimum number of radial basis states.

BUTTLE = 4 for none, 0,2 for complex, 1,3 for real (2,3 without energy shift) Buttle correction (default 0)

PRALPHA = print basis-state eigenvalues to files fort.60,61,62,63

PCON = trace variable for calculation of radial basis states (same meaning as IPC on Cards 13 for single-particle bound states).

MEIGS = maximum number of bound states to find, if ENLAB < 0 on Card 19.

RMATR = R-matrix matching radius (default is RMATCH on Card 1). Warning: RMATR will be changed to an even multiple of HCM.

EBETA(i) = energy  $\hbar^2 k^2 / 2m$ , where  $k = f' / f$ , the logarithmic derivative for all radial basis states at  $r=RMATR$ , with  $k$  having the same sign as EBETA(i). Use i=1,2 for positive,negative parity coupled channels sets (respectively).

If R-matrix solutions are selected (by IBLOCK<0) then all channels are 'blocked' together and solved in a full CRC procedure.

If WEAK>0, then non-elastic columns of the R-matrix are set to zero, when penetrabilities < WEAK.

## 2.2 Trace Control Variables:

#### Card 5

```
14I2
CHANS, LISTCC, TRENEG, CDETR, SMATS, XSTABL, NLPL, WAVES, LAMPL, VEFF, KFUS, WDISK,
BPM, MEL, CDCC, NFUS
```

A value of 0 gives no trace, increasing values give progressively more printed output.

*Decrement*ed variables are decreased by 1 on each use.

CHANS ≥ 1 : Print the sets of coupled partial waves for each J,parity. Decrement.

LISTCC

= 1 : Print coupling coefficients between these channels. Decrement.

= 1,2,... Print progressively more detail of couplings.

TRENEG

≥ 1 : Print all potentials as they are calculated from Cards 10

≥ 3 : Print all potentials as they are calculated from Cards 9

CDETR

≥ 1 : Print information on the solving of the coupled equations. (decrement).

SMATS

≥ 1 : Print absorbtion & reaction cross sections for successive partitions and excitations.

$\geq 2$  : Print elastic S-matrix elements ( $S_{el}$ ). Also ‘punch’ these elastic  $S_{el}$  on output file 7, in format (2F15.10,L,J,JTOT) for  $S_{el}$  complex, L, J and JTOT. See WDISK below for description of these quantum numbers.

$\geq 3$  : Print all S-matrix elements for the ‘grazing partial waves’ defined by  $0.05 < Re(S_{el}) < 0.95$

$\geq 4$  : Always print all the S-matrix elements.

$\geq 5$  : Print all S-matrix elements at each iteration of the coupled equations (or, if PADE  $> 0$ , the Pade approximant)

$\geq 6$  : Print all actual S-matrix elements at each iteration (these may be divergent before Pade acceleration).

XSTABL  $\neq 0$  : If XSTABL is non-zero, in file 16 punch output cross sections for all excitation levels in all partitions. A header card in FORMAT(5I6) gives partition IC, level pair IA, number of tensor ranks of analysing powers  $1 < KQ1PR < XSTABL$ , number of angles NANGL, and NEARF. NEARF=1 for total cross section, 2 for far-side component, and 3 for near-side component.

Then follow NANGL print operations in FORMAT(1P, 6E12.4), repeating the FORMAT for each operation if KQ1PR is large, of THETA, elastic xs (mb),  $T_{10}$ ,  $iT_{11}$ ,  $T_{20}$ ,  $T_{21}$ ,  $T_{22}$ ,  $iT_{30}$ ,  $iT_{31}$  etc.

NLPL  $> 0$  : print a ‘contour plot’ of the non-local kernels  $K_{fi}(R_f, D_{fi})$ . This is useful to determine if the parameters on card 1 are adequate. Decrementd.

#### WAVES

$\pm 1$  or  $\pm 3$  : print out wave function solutions of the coupled equations at the end of the iterations. (If WAVES  $< 0$  : print out the RATIO of the w/f to its asymptotic form  $((G - iF) - S.(G + iF)).i/2$ )

2 or 3 : print out the source terms at *each* iteration of the coupled equations.

#### LAMPL

$\neq 0$  : Print out (on Fortran file 36) the coefficients  $A(m'M' : mM; L)$  for the Legendre coefficients in the scattering amplitude for the partition number abs(LAMPL), and print out the  $f(m'M' : mM; \theta)$  for each angle  $\theta$ .

$< 0$  : only print out on file 37 the amplitudes  $f$ , not the A’s, for partition abs(LAMPL).

The phase convention here is that there is no Coulomb phase shift for  $L = 0$  in the Coulomb scattering amplitude : factors such as  $\exp i(\sigma_L - \sigma_0)$  appear in the A’s.

#### VEFF

$\neq 0$  : Calculate the ‘coupled channels effective potential’ found by averaging the ‘trivially equivalent potential’ over all the  $J, \pi$  sets, with weights of the elastic wave functions times the reaction cross section, in each set.

$< 0$  : Add this effective potential to optical potential of the elastic channel before printing.

= -2 or +2 : Exclude partial waves with elastic S-matrix element  $S_\ell < 0.1$  from the averaging sum.

The results show the real and imaginary parts for successive values of  $J - L$ , for the projectile only.

#### KFUS,NFUS

$> 0$  : Calculate ‘core fusion’ using the imaginary and scalar parts of potential number KFUS (i.e. cards 10 with TYPE = 1 or 2, and KP = KFUS), also for the first NFUS inelastic channels

#### WDISK

= 1 : Print elastic wave functions on output file 17, FORMATTED

= 2 : Print all wave functions on output file 17, FORMATTED

= -1 : Print elastic wave functions on output file 17, UNFORMATTED

= -2 : Print all wave functions on output file 17, UNFORMATTED

The following data formats are used when WDISK  $> 0$  :

card A: (I4, 2F8.4, F8.1, I3)

NR, H, ENLAB, JTOTAL, PARITY, MP, MT, ZP, ZT :  
 number radial points, step size, lab. energy, J, pi,  
 projectile and target masses and charges  
 card B: (2I4, 2F6.1, I4, F6.1, 2F15.10, f12.8)  
 IT, L, J, JTOT, LIN, JIN, SMAT (complex), ETA

where

IT = index to excited state pair, counts cards 7.

L = partial wave

J = L + projectile spin

JTOT = total spin =  $J_{total}$  = J + target spin

LIN = incoming partial wave

JIN = incoming J value.

SMAT = S matrix element for this partial wave.

card C: (6E12.4) (psi(I), I=1, NR) wave function

card C is repeated until NR complex values given

NB: the first point psi(1) = 0 always, as at r=0

Cards B & C are repeated for each channel, until IT < 0.

When WDISK < 0, successive records contain the two real values of psi(I), starting IN THIS CASE, from I=2 (i.e.  $r = h$ ).

## BPM

≥ 1 : Calculate fusion cross sections in the Barrier Penetration Model using first the bare potential, and then the bare potential + the ‘weighted equivalent potential’ calculated when  $VEFF \neq 0$ .

≥ 2 : Print out L-distributions of the fusion cross section.

MEL – ignored

## CDCC

≠ 0: Print out the  $f(m'M' : mM; \theta)$  for each angle  $\theta$  on file 57 for partition PEL, after the following information:

card A: (F10.4, 3F8.4) ENLAB, Bproj, H2SM, e^2 lab energy, projectile binding energy  
 hbar^2/2.m, e^2  
 card B: (4f8.4) massp, masst, massc, massv masses projectile, target, core, valence  
 card C: (4f8.4) Zp, Zt, Zc, Zv charges  
 card D: (4A8) namep, namet, namec, namev names  
 card E: (4f8.1) Jp, Jt, Jc, Jv g.s. spins  
 card F: (4i8) Pp, Pt, Pc, Pv g.s. parities  
 card G: (4I4) NBINS, NKMAX, NEXB, NNJMAX no. CDCC bins, max NK,  
 no. excited states, max(2\*Jex+1)  
 card H: (I4, 2f8.4) NANGL, THMIN, THINC (cm angular range from Card 3)  
 for each of the NBINS bins:  
 card I: (i2, 2f4.1, 3f8.4, 2i4)  
 l, j, Emid, kmin, kmax, NK, KN, ISC  
 l, j: quantum numbers (s==Jv)  
 Emid: centre of bin with respect to continuum threshold  
 kmin, kmax, NK: Min, max and number of k values in bin integral  
 KN: original KN index for bin state  
 ISC: normalisation used for bin



```

for each IK=1,NK
  card J: (10f8.4) delta(IK): nuclear phase shift used in bin integral (radians)

for each excited state pair in the entrance partition: IA=1,NEXB::
  card K: (f4.1,i4,f8.4,i4) Jex,Parity,Eex,IBIN:
    Jex :          spin of this projectile excited state
    Parity:        parity of this projectile state
    Eex:           excitation energy of this state above g.s.
    IBIN:          (first) bin defined for this excited state
  for each IANG=1,NANGL: read complex numbers:
    card L: (6E12.4): ((FAM(MEX,MP,IANG,IA),MEX=1,2*Jex(IA)+1),MP=1,2*Jp+1)

```

The phase convention again is that there is no Coulomb phase shift for  $L = 0$  in the Coulomb scattering amplitude : factors such as  $\exp i(\sigma_L - \sigma_0)$  appear in the  $A$ 's.

Summary of bin normalisation factors for different ISC values:

ISC

$$\begin{aligned}
&= 2: \exp(-i\delta(k)) \\
&= 4: \sin(\delta(k)) \exp(-i\delta(k)) \\
&= 12: k \exp(-i\delta(k)) \\
&= 14: k \sin(\delta(k)) \exp(-i\delta(k))
\end{aligned}$$

## 2.3 Partitions and Excited States

### Card 6

(for each partition IC=1,2,... repeat until a blank card 8) :

```
A8,          2F8.4,          I4,    L1,1X, A8,          2F8.4,          F8.4
NAME(1, ), MASS(1, ), ZZ(1, ), NEX( ), PWF( ), NAME(2, ), MASS(2, ), ZZ(2, ), QVAL(IC)
```

```
name-----mass-----charge-          name-----mass-----charge-
----projectile-----          -----target-----
```

Abs(NEX) = number of pairs of excitations of projectile and/or target,

PWF = T, if acceleration of long-range Coulomb couplings to be performed when card 1a present. Default is T.

QVAL =  $Q$  value of this partition, relative to the  $Q$ -values of the other partitions, for  $E_p = E_t = 0$ .

If NEX < 0, then cross sections for this partition are not printed.

### Card 7

(repeat NEX times before the next Card 6) :

```
F4.1, I2,    I2,    F8.4, 2F4.1, I4, 1X, A1
Jp,  COPYp, BANDp , Ep,  KKp, Tp, KP, PWF,
-----projectile state-----
```

```
F4.1, I2,    I2,    F8.4, 2F4.1,  2L2,          2I4
Jt,  COPYt, BANDt , Et,  KKt, Tt, EXCH, IGNORE, INFAM, OUTFAM
-----target state-----
```

This card is repeated NEX times, IA=1,NEX

For both projectile (p) and target (t), the following are read :

J = spin of the state

BAND > 0 for positive parity state, and < 0 for negative parity. The value of BAND defines the rotational band : all states of the same BAND may be coupled by rotational mechanisms.

If COPY is positive, then this level is a copy of a previous level number (COPY < IA) in the same partition.

If COPYp < 0, then this level is an exchange copy of *the same IA numbered* level in the previous partition abs(COPY). That is, a copy with projectile and target nuclei exchanged.

If COPYt = -IC, then the target state is an exchanged projectile. If that state has spin zero, then only even partial waves are allowed.

COPYs are needed to define identical states of one nucleus in different pairings IA. Spectroscopic amplitudes (see Cards 17) should be defined for only the original 'copied' level.

E = excitation energy of state relative to ground state.

KK = K of rotation band containing this state. (If zero, use spin of first level in this band.)

T = isospin of this state (if zero, use INT((mass-2\*charge)/2)) (The T value is not used by this version of FRESCO).

KP = index of optical potential for this pair of excited states.

PWF= T to use CRCWFN coupled Coulomb wave functions in this partition (see Cards 1,1a)

If zero, use as default KP = IC, the number of this partition.

If EXCH = T calculate and write out all cross sections and amplitudes for  $180 - \theta$ .

If IGNORE = T, ignore the convergence of this state pair (see IPS discussion on Card 4).

If INFAM  $\neq 0$ , read in complex amplitudes later to add to calculated scattering amplitudes (see cards A3). (If INFAM  $< 0$ , read in only one amplitude (non spin-flip) for each scattering angle.)  
If OUTFAM  $\neq 0$ , write out complex amplitudes later to add to calculated scattering amplitudes (see cards A3). (If OUTFAM  $< 0$ , write out only one amplitude (non spin-flip) for each scattering angle: the average of diagonal amplitudes.)

### Card A3

Cards A3 : Extra scattering amplitudes –

If INFAM on a Card 7 is non-zero, then read on file |INFAM|, on a new card for each scattering angle, some complex amplitudes  $f(\theta)$ , to be added to those calculated by the program before the cross sections are calculated.

If INFAM  $< 0$ , then only *one*  $f(\text{external})$  is read, and this is used for all the diagonal  $f(mM:mM)$ , the off-diagonal values being zero.

If INFAM  $> 0$ , then all the  $f(m'M' : mM)$  are read in.

### Card 8

Blank card for end of reading partitions.

## 2.4 Potentials

Cards 9,10 (to define the potentials to be indexed by KP) :

Each potential is defined by a Card 9, defining the radii to be used and the diagonal Coulomb potential, followed by any number of Cards 10 which cumulatively construct the components of the nuclear potential. The first input on each card is KP, identifying the potential of which this is to be a component.

### Card 9

Card 9: I3,I2,3X,2F8.4, 2F8.4  
 KP, 0, A#1,A#2, R0C,AC (i.e. would be Card 10, but TYPE=0)

All the radii are multiplied by CC, which is updated by a TYPE=0 Card 9 to  $CC = A\#1^{1/3} + A\#2^{1/3}$  and by TYPE>0 Cards 10, if  $P0 > 0$ , to  $CC = P0^{1/3}$

R0C = radius (when multiplied by CC) of charge distribution

AC = diffuseness of charge distribution

The values of A#1 and A#2 affect *only* the conversion from  $r_0$  radii to R radii in the definition of potentials in Cards 9 & 10. If however you adopt the convention that A#1 is the target mass number and A#2 the projectile's, then FRESCO can later display the fractional  $\beta$  values corresponding to given deformation lengths. (These are for information only, and do not affect the couplings.)

### Card 10

Card 10: I3,I2, A1,I2, 3F8.4, 3F8.4, F8.4  
 KP, TYPE, IT, SHAPE, P1,P2,P3, P4,P5,P6, P0  
 ---REAL--- -IMAGINARY- A#  
 V,Vr0,Va, W,Wr0,Wa, A#

for TYPE

1	SHAPE	Central potential, Volume
2	SHAPE	Central potential, Derivative (i.e. surface)
3	SHAPE	Spin-orbit for projectile
4	SHAPE	Spin-orbit for target
5	SHAPE	Tr tensor force for projectile
6	SHAPE	Tr tensor force for target
7	SHAPE	Tensor force between L and combined projectile+target spins (e.g. n-p tensor force)
8	SHAPE	Spin.spin force for target & projectile spins
10	SHAPE	Deformed projectile (matrix elements from ROTOR)
11	SHAPE	Deformed target (matrix elements from ROTOR)
12	SHAPE	Projectile coupled by matrix elements read in.
13	SHAPE	Target coupled by matrix elements read in.
30	SHAPE	L(L+1) central potential, Volume
0	-	Coulomb potential : see Card 9.

Where TYPE indicates type of spin tensor or excitation coupling,

IT is '1' or '3' to make this component included only iteratively,

'2' or '3' to NOT subtract this component in KIND=3,4 single-particle couplings,

the SHAPE indicates the radial shape of the form factor,  
and P1-P3 & P4-P6 are parameters for the real and imaginary parts (respectively).

If TYPE < 0, add new potential numerically into previous potential, and use abs(TYPE) instead. This saves space, and is necessary if adding together components to be deformed by a following card  $10 \leq \text{TYPE} \leq 13$ .

If KP < 0, this will be the last Card 10. Use abs(KP) below, and omit Card 12.

The SHAPEs for volume potentials (TYPE=1, 8 & 30) are,  
with  $R = P2 * CC$ ,  $RH = (r - R)/P3$ , and  $E = \exp(-(r-R)/P3)$ ,  
(replacing (P1,P2,P3) by (P4,P5,P6) throughout for the imaginary parts)

- 0: Woods-Saxon =  $- P1 / (1 + 1/E)$
- 1: WS squared =  $- P1 / (1 + 1/E)^2$ .
- 2: Gaussian =  $- P1 * \exp(-RH^2)$ .
- 3: Yukawa =  $- P1 * E / r$
- 4: Exponential =  $- P1 * E$
- 5: Reid soft core for  $T=0$ , central part
- 6: Reid soft core for  $T=1$ , central part
- 7: Read Real
- 8: Read Imaginary
- 9: Read Complex
- 1: Fourier-Bessel =  $j_0(RH) = \sin(RH)/RH$

For 'SHAPE's 7-9, immediately read in a comment card, then (free format) NPOINTS, RSTEP, RFIRST, followed by NPOINTS potential points for the shape in steps of RSTEP starting at  $r=RFIRST$ , reading card images all from *Input File 4* in free format.

Rescale the real part by P1, the imaginary part by P2, and use radius =  $P3 * CC$  for subsequent deformation calculations.

If SHAPE = -7, -8, or -9, rewind file 4 before reading from it.

The SHAPEs for surface potentials (TYPE=2), with R, RH and E as before, are the first derivative forms (normalised to -1 when  $E=1$ , if reasonable):

- 0 : Woods-Saxon =  $- P1 * 4 * E / (1+E)^2$
- 1 : WS squared =  $- P1 * 8 * E * E / (1+E)^3$
- 2 : Gaussian =  $- P1 * 2 * \exp(-RH * RH) * RH$
- 3 : Yukawa =  $- P1 * E * (1 + r/P3) / (r * r)$
- 4 : Exponential =  $- P1 * E$
- 5 : Reid soft core for  $T=0$ , spin-orbit part  $\times r$ ,
- 6 : Reid soft core for  $T=1$ , spin-orbit part  $\times r$ ,
- 7,8,9 : Read from cards, as above.

The SHAPEs for spin-orbit potentials (TYPE=3 or 4) are the following surface shapes,  
where  $CONLS = \hbar^2 / (m_\pi^2 c^2) = 2.000$ .

- 0 : Woods-Saxon =  $- CONLS * P1 * E / [(1+E)^2 * P3 * r]$
- 1 : WS squared =  $- CONLS * P1 * E * E / (1+E)^3 / (2 * r * P3)$
- 2 : Gaussian =  $- CONLS * P1 * \exp(-RH * RH) * RH / (2 * r * P3)$
- 3 : Yukawa =  $- CONLS * P1 * E * (1 + r/P3) / (4 * r^3 * P3)$
- 4 : Exponential =  $- CONLS * P1 * E / (4 * r * P3)$
- 5 : Reid soft core for  $T=0$ , spin-orbit part

6 : Reid soft core for  $T=1$ , spin-orbit part

7,8,9 : Read from cards, as above.

To become interaction potentials, these form factors will be multiplied by  $j(j+1) - l(l+1) - s(s+1) = 2\mathbf{l} \cdot \mathbf{s}$ , where  $s$  = spin of projectile or target in each of its ground state and excited levels. There is no option here for state-dependent spin-orbit forces.

The SHAPes for tensor potentials (TYPE=5, 6 & 7), with R, RH and E as before, are the second derivative forms (normalised to unity when  $E=1$ , if reasonable):

0 : Woods-Saxon =  $P1 * 8 * E * (E-1) / (1+E)^3$

1 : WS squared =  $P1 * 4 * E * E / (1+E)^3$

2 : Gaussian =  $P1 * 2 * \exp(-RH * RH) * RH$

3 : Yukawa =  $P1 * E * (1/P3^2 + 2/r^2) / r$

4 : Exponential =  $P1 * E$

5 : Reid soft core, 12 \* tensor part

6 : Vol Gaussian =  $12 * P1 * \exp(-RH * RH)$

7,8,9 : Read from cards, as above.

If  $SHAPE \geq 30$ , then use SHAPE-30, and define a  $J$ - or  $L$ -dependent potential by a factor defined by reading in Card 10.5:

Card 10.5      4X,A1,I3,2F8.4              JL,LSHAPE,XLVARY,ALVARY

so that the potential is multiplied by a form factor:

LSHAPE=0 : Woods-Saxon =  $1 / (1 + 1/E)$ ,

=1 : WS squared =  $1 / (1 + 1/E)^2$

=2 : Gaussian =  $\exp(-RH^2)$ ,

where  $X=L$  (for  $JL='L'$ ),  $X=J$  ( $JL='J'$ ),  $RH = (X-XLVARY)/ALVARY$ , and  $E=\exp(-RH)$ .

If  $SHAPE \geq 10$  and  $< 19$ , then use SHAPE-10, and write out the resulting potential to *Output file 25* in FORMAT(6E12.4): a form suitable for subsequent reading by a  $SHAPE \geq 20$ .

If  $SHAPE \geq 20$  and  $< 30$ , then a  $J_T/\pi$ -dependent potential is defined.

For each subsequent coupled-channels set with total angular momentum  $J_T$ , a form factor is read into this potential from *Input file # SHAPE*, reading  $M = RMATCH/HCM+1$  complex numbers in FORMAT(6E12.4) from the file as a random-access set of card images, with  $(M-1)/3+1$  card images for each form factor.

For each CC set, form factor number  $\text{int}(J_T) + 1$  (for  $SHAPE \geq 24$ ) or 1/2 for  $\pm$  parity (for  $SHAPE < 24$ ) is read.

If  $SHAPE = 40$ , then a  $\pi$ -dependent potential is defined: use  $KP = P1$  for  $+$  parity CC sets, and  $P2$  for  $-$  parity.

If  $SHAPE = 41$ , then a  $L$ -dependent potential is defined: use  $KP = P(L+1)$  for  $L=0-5$ , and  $P0$  for  $L \geq 6$ .

If  $SHAPE = 42$ , then a  $J$ -dependent potential is defined: use  $KP = P(J+1)$  for  $J=0-5$ , and  $P0$  for  $J \geq 6$ , with  $J = \text{int}(J_T)$ .

If  $SHAPE = 43$ , then a  $L$ -parity-dependent potential is defined: use  $KP = P1$  for  $L$  even, and  $P2$  for  $L$  odd.

There need only be one Card 9 or 10 for  $40 \leq SHAPE \leq 43$ . The values of TYPE and P2-P7 are ignored.

No files are used. Choices are listed in fort.48

If  $SHAPE = 45$ , then an energy-dependent potential is defined, using linear interpolation of the potential forms.

The nodes are  $KP=P1$  at energy  $P2$ ,  $P3$  at energy  $P4$ , etc., up to  $KP=P9$  at energy  $P10$  (MeV).

### Nucleon - nucleon Potentials

The SHAPes for the nucleon-nucleon SSC (C) potential (TYPE = 8) are taken from the subroutine SSCC in FRESKO. The input NUM is the number of angular momentum components stored, using the order  $^1S_0, ^3S_1, ^3S-^3D, ^3D_1, ^1P_1, ^3P_0, ^3P_1, ^3P_2, ^3P-^3F, ^3F_2, ^1D_2$ , and  $^3D_2$

Note that TYPEs 8 & 9 can only be used in KIND = 1 (LS-coupled) single-particle states.

The SHAPes for the user's nucleon-nucleon potential (TYPE = 9) are taken from the subroutine NNPOt, with NUM the same meaning as above.

### Deformations

The SHAPes for deformed potentials (TYPE  $\geq 10$ ) are constructed either by reading external forms (SHAPE = 7, 8 or 9) for each P(k) non-zero (the input k-form being multiplied by P(k)), or (for SHAPE  $\geq 10$ ) by deforming the potential on the *immediately preceding* input card. This preceding card must be of TYPE=0 for Coulomb deformations, or TYPE = 1 or 2 for nuclear deformations: deformation of non-central forces is not yet implemented.

For Nuclear deformations P(k) = DEF(k), the deformation lengths (in fm.). (P0 = DEF(0) for *inelastic* monopoles.)

For Coulomb deformations P(k) = Mn(Ek), the intrinsic reduced matrix elements in units of  $e.fm^k$  (P0 gives Mn(0) for *inelastic* monopoles). These intrinsic matrix elements Mn(Ek) use the reduced matrix elements  $\langle I' || Ek || I \rangle$  given by the definitions of Alder & Winther (not by those of Brink & Satchler), by assuming a rotational model where K is a good quantum number:

$$Mn(Ek) = \langle I' || Ek || I \rangle / (\sqrt{2I+1} \langle IKk0 | I'K \rangle) .$$

Thus, for (possibly hypothetical)  $0 \rightarrow k$  transitions,  $Mn(Ek) = \langle k || Ek || 0 \rangle$ .

Mn(E2) is related to the intrinsic quadrupole moment in the rotational model by  $Mn(Ek) = Q_0 \sqrt{5/16\pi}$ . For a uniformly charged sphere of radius R, to first order in  $\beta_k$  we have

$$Mn(Ek) = \frac{3 Z \beta_k R^k}{4\pi} .$$

The Mn(Ek) are thus of the same sign as  $\beta$  and  $Q_0$  for all rotational bands.

TYPES 12 & 13, for detailed and model-independent specifications, directly use the reduced matrix element

$$\begin{aligned} M(Ek) &= i^{I'-I+|I-I'|} \langle I' || Ek || I \rangle \\ &= \pm \sqrt{(2I+1) B(Ek, I \rightarrow I')} , \end{aligned}$$

where the sign convention has been chosen to make M(Ek) real and symmetric under  $I \leftrightarrow I'$  interchange. The diagonal reduced matrix element gives the spectroscopic quadrupole moment

$$Q_2 = \sqrt{16\pi/5} (2I+1)^{-1/2} \langle II20 | II \rangle \langle I || E2 || I \rangle .$$

The intrinsic and reduced matrix elements are therefore connected by

$$M(Ek) = Mn(Ek) (-1)^{[I-I'+|I-I'|]/2} \sqrt{2I+1} \langle IKk0 | I'K \rangle$$

in the rotational model where K is a good quantum number, for states of spin I, I', projection K, charge Z, and radius R (DEF(k) =  $\beta_k \times R$  for such states).

So Mn(Ek) is the square root of  $B(Ek, 0 \rightarrow k)$  with some sign within  $K = 0$  bands. Mn(Ek) always has the same sign as  $\beta$ .

IN OTHER CASES, DO **NOT** ASSUME THAT ALL TRANSITIONS HAVE THE SAME  $M(Ek)$  VALUES. *THUS  $Mn(Ek)$  ARE THE SAME FOR ALL PURE ROTOR TRANSITIONS, IN CONTRAST TO  $M(Ek)$ .* In order to guide the user here, effective  $\beta$  values are calculated from the given  $Mn(Ek)$  or  $M(Ek)$ , for each possible transition. *From version FRV onward,  $Mn(Ek)$  is used in place of  $M(Ek)$  for TYPE 10 & 11 potentials.*

## Card 11

For TYPEs 12–13, Cards 11 are read to determine the details of the required couplings between each pair of excited states and of the reorientation terms for each individual state.

Card 11            4X, 3I4, F8.4            IB, IA, k, STR

to put in a coupling *to* state IB *from* state IA, of multipolarity k and strength STR. Note: monopole potentials are included automatically, even if not listed here.

For each k used here, P(k) must have been non-zero, and the required coupling has the same form factor but with relative strength STR / P(k). That is, STR is the reduced matrix element  $\langle IB | M(Ek) | IA \rangle = M(Ek, IA \rightarrow IB)$  for Coulomb transitions (**NOT**  $Mn(Ek)$ ), and is the ‘*reduced* deformation length’ RDEF(k) for nuclear transitions.

This ‘reduced deformation length’ in the rotational model is

$$\begin{aligned} RDEF(k, I \rightarrow I') &= DEF(k) (-1)^{[I-I'+|I-I'|]/2} \sqrt{2I+1} \langle IKk0 | I'K \rangle \\ &= M(Ek) * 4\pi / [3ZR^{k-1}] \end{aligned}$$

but may in general be varied independently of DEF(k) and M(Ek). Both these nuclear and Coulomb interactions are thus designed to give channel couplings which are *independent* of the projection K values read in the Cards 7. This of course requires making RDEF(k) and M(Ek) dependent on the spins of the excited states, not on any simple model.

The SHAPES for deformed potentials (TYPE=10 to 13) are constructed by:

SHAPE = 0 to 6 : not used (as card gives deformation strengths).

= 7,8,9 : Read from cards, as above for TYPE=1. The multipoles are then multiplied by P(k) (by 1.0 for k=0), and should end up as scaled to replace the form factors calculated below:

= 10 : Coulomb multipoles have the usual simple form for a deformed charged sphere to produce  $M(Ek) = P(k)$ , varying at large distances as

$$F(r) = M(Ek) e^2 \frac{\sqrt{4\pi}}{(2k+1)} r^{-k-1}$$

where  $e^2 = 1.440$ , and where this form factor will later be multiplied by the charge number of the opposing nucleus.

= 10 : Nuclear multipoles are the deformation length  $DEF(k) = P(k)$  times the derivative of the undeformed potential times  $-1/\sqrt{4\pi}$ :

$$F(r) = -DEF(k) \frac{1}{\sqrt{4\pi}} \frac{dU(r)}{dr}$$

The shape is the same for all multipoles  $k > 0$ .

= 11: Nuclear multipoles calculated by numerically deforming the radii of the previous potential, and



projecting by Gaussian quadrature onto the required multipoles (those  $k > 0$  for which  $P(k)$  is non-zero). For small deformation lengths, these SHAPes are the same as for SHAPE = 10.  
= 12: Same as SHAPE = 11, except that the monopole  $k = 0$  part of the potential is also recalculated by quadrature. A first order correction is made to the radius to improve volume conservation.  
= 13: Same as SHAPE = 12, except that **no** first order correction is made to the radius to improve volume conservation.

## Card 12

Blank card for end of reading potential parameters.  
(Unless the last KP on card 10 was negative)

## 2.5 One- and Two-Particle Form Factors

Read in a card for each desired particle-nucleus form factor, then a blank card (13).

Each form factor is indexed by a number KN, which may refer to a single form, or for two-nucleon form factors will refer to a range of forms KN1 - KN2 (one for each distance and angular momentum between the two nucleons).

Each form factor is the binding of one or two particles to a specified nucleus, where the composite system is another specified nucleus.

To specify the core and composite nuclei, their partition numbers IC1 and IC2 are required (either order), with  $|IN|=1$  for projectile and  $|IN|=2$  for target nuclei.

The mass of the particle is the strict difference of the masses of the core and composite nuclei, except that if  $IN < 0$ , then a relativistic correction is made for effect of the relative Q-values on the mass of the composite nucleus, when extracting by differences the mass of the bound fragment.

### Card 13

```

2I3,      3I2,      I2,  1X,A1,  3I2,      F4.1,I2,F4.1,I2,
KN1,KN2,  IC1,IC2,IN, KIND,    CH1,  NN,L,LMAX,SN,IA,JN,IB

2I3,      F8.4,  2I3,      I3,  I3,F8.4,  I3,3F8.4
KBPOT,KRPOT, BE,    ISC,IPC, NFL,  NAM,AMPL, NK,ER,RSMIN,RSMAX,

f8.3,      i4,      F8.3
RSALPHA,NLAG,PHASE

```

where

KN (=KN1) or the range KN1-KN2 indexes this form factor,

IC1, IC2, IN define the particle and core nuclei as explained above,

KIND is the kind of couplings:

= 0 for (LN,SN) JN couplings ← use for typical transfers

= 3 for  $|(LN,SN)J_n,J_{core};J_{com}\rangle$  (IA & IB must be given)

= 6 for  $|L_{nn},(\ell,S_{12})j_{12};J_{12}\rangle$  with isospin  $(.5,.5)T=9$  for  $(L_{nn},(\ell,S_{12})j_{12})J_{12},J_{core};J_{com}\rangle \& (.5,.5)T,T_{core};T_{com}$

where

$J_{core}$  = spin of core nucleus (state Ia if given)

$J_{com}$  = spin of composite nucleus (state IB if given)

CH1 = single-character identifier to distinguish clusters of nucleons of different structures that are not further described but should not be confused with each other. Use A-M for positive parity clusters, and N-Z for negative parities.

NN = number of nodes (include the origin, but not infinity, so  $NN > 0$ )

L = LN = angular momentum of bound cluster relative to the core

LMAX = maximum value of L in states in deformed potential,

SN = intrinsic spin of bound nucleon (one-particle states)

= total angular momentum (L+S) of bound cluster (KIND 9)

IA = index (within core partition) of excited state of core, or zero if to be specified later.

JN = vector sum LN + SN

IB = index (within composite partition) of excited state of composite, or zero if to be specified later.

KBPOT = index KP of potential in which to bind this state

KRPOT = index KP' of potential with which to multiply this states' wave function for transfer interactions.

If zero, use KBPOT. If the binding potential was adjusted for a specific binding energy, then this adjusted potential (not the original) is used for transfers.

BE = Binding Energy (positive for bound states, negative for continuum bins)

RSMIN,RSMAX = After calculation, radial wave functions are set to zero for radii below RSMIN and/or above RSMAX. No further renormalisations are performed.

RSALPHA = After calculation, radial wave functions are rescaled by radial factor  $e^{-\alpha r}$  for  $\alpha = \text{RSALPHA}$ . No further renormalisations are performed.

NLAG= Use Lagrange mesh to find bound states, with NLAG basis functions.

PHASE= Find potential to give phase shift of PHASE degrees at energy  $-BE$  for bins. Requires  $NLAG \gg 0$ .

The revised potential is saved for further bins, just as with  $ISC < 0$  for bound states.

### BOUND STATES:

ISC = 0 to vary the binding energy for fixed potential,

> 0 to vary the TYPE = ISC component of the potential KBPOT by a scaling factor to give binding energy BE.

< 0 to vary the TYPE = ISC component of the potential KBPOT, as above, but **also** to permanently rescale all the varied potential components. This affects all later bound and scattering states using the potential KBPOT.

### CONTINUUM BINS:

ISC (default value 2)

= -2: no weighting or normalisation,

= 1,2 : weight wave functions by  $\exp(-i\delta(k))$ , so they are real, before integrating over bin width.

= 3,4 : weight wave functions by  $T(k)^*$  (useful for resonances)

= -1,1,3 : normalise wave functions to unity (by usual square norm). **(This option is not recommended, for physics reasons!)**

$\geq 10$ : use additional  $k$  factor in the weighting function, with  $\text{mod}(\text{ISC}, 10)$  for above choices. Recommended for low-energy bins.

The values  $ISC > 0$  give real-valued bins for single-channel states, but not, in general, for coupled-channels bins.

In that case, Fresco stores *all* bound and continuum states as complex functions.  $\text{KIND}=3$  and 4 forward and reverse couplings are both calculated explicitly, but not  $\text{KIND}=7$  transfer couplings. For transfers, the reverse couplings must be put in explicitly.

**Warning:** imaginary parts of bins give imaginary parts of long-range Coulomb couplings that are *ignored* between  $\text{abs}(\text{RMATCH})$  and  $\text{RASYM}$  in the  $\text{CRCWFN}$  calculations (the values on Card 1a).

In general,  $ISC=2$  is recommended (or  $ISC=4$  for resonances), since then the coupled-channels bins will be nearly real. With  $ISC=-2$  (no phase weighting) there will be different results because of different weighting within the bin. Note that all channels within a bin have the same scalar weighting factor.

IPC = print control for further infomation:

IPC	Print Iterations	Print Final Result	Print W/F
0	no	no	no
1	no	yes	yes
2	no	yes	no
3	yes	yes	yes
4	yes	yes	no

For bin states, read this table with ‘iterations’ replaced by ‘intermediate phase shifts’.

NFL < 0 : to write wave-function  $u(R)/R$  and potential overlap  $V(R)u(R)/R$  to file number  $\text{abs}(NFL)$ .

> 0 : to read a previously-written wave function from file number NFL.

These wave function files contain a comment card, then (free format) NPOINTS, RSTEP, RFIRST, followed by NPOINTS wf points in steps of RSTEP starting at  $r=RFIRST$ , and then NPOINTS for the vertex function (potential\*wf). The file numbers NFL should be in the range 20–33 (see appendix IV).

NAM, AMPL = if IA and IB are both non-zero, then there is enough information to set up the spectroscopic amplitude now, to  $\sqrt{NAM} \times AMPL$ . See Card 17, and discussion after Card 15, for further information about these amplitudes.

**Note:** If this is a form factor with mixed core levels, then AMPL should be specified *here* rather than on a Card 17 (as Card 17 requires an IA specification, and such a state would have multiple IA assignments).

If NAM = -1, then use AMPL for the mass of the bound particle, independent of the MASSES on Cards 6. (If  $NAM \geq 0$ , then the default particle mass is the difference of the MASSES of the projectiles (IN=1) or targets (IN=2) for partitions IC1 and IC2).

If NAM < -1, then use AMPL instead of ERANGE for the range ER of the energies of the upper and lower boundaries of the continuum bins, and use at least  $NK=5 \times |NAM|$  integration steps over this range. (These ER and NK override the input values.)

### 2.5.1 One-particle KINDs

For KIND = 0, (LN,SN) JN couplings.

One form factor with LN,SN, & JN as read in.

LMAX is not used.

IA & IB are used only if NAM & AMPL are non-zero, to specify spectroscopic amplitudes.

For KIND = 3, sum over coupled core and (ls)j particle states :

Coupled form factors  $(L_n, SN)J_n, J_{core}; J_{com}$  (summing over  $L_n, J_n$  &  $J_{core}$ ).

NN is the required number of radial nodes for the component wave function with core state IA and partial wave  $L_n = L$ .

LMAX is maximum  $L_n$  in summation.

SN as read in, the intrinsic spin of the bound particle.

All core states are included that can be coupled to form  $J_{com}$ , using a deformed binding potential.

*Note that such a deformed potential must be TYPE = 11, whether the projectile or target is deformed: not 10 or 12 or 13.*

JN is the maximum  $J_n$  in the summation (single particle  $l + s$ )

IB gives  $J_{com}$  (fixed) : spin of composite nucleus.

BE is the single-particle binding energy for core state IA.

### 2.5.2 Two-particle KINDs

For KIND  $\geq 6$ , two-particle bound states are constructed out of sums of pairs of previously-defined one-particle states, and input parameters NN through to BE on Card 13 are given new meanings.

NN  $\rightarrow$  NPAIRS, the number of pair-products to be summed

$L \rightarrow \ell_{min}$  , minimum orbital angular momentum  $\ell$ .

$LMAX \rightarrow \ell_{max}$  , maximum orbital angular momentum  $\ell$ .

$SN \rightarrow S_{min}$  , minimum sum  $S_{12}$  of the two nucleons' intrinsic spins ( $S_{max} = 1.0$  always).

IA, IB give core and composite states, as before.

$JN \rightarrow J_{12}$  , total angular momentum of the two-particle state outside  $J_{core}$ .

$KBOT \rightarrow T$  , total Isospin of the 2-nucleon state (0 or 1)

(used to enforce  $\ell + S_{12} + T = \text{odd}$ )

$KRPOT \rightarrow KNZR$ , the KN index to a single-particle state  $u_{12}(r)$  of KIND 0 or 1, giving the N-N relative motion in the other participating nucleus (usually in the light ion).

If  $KNZR > 0$ , then just the overlap  $u(R) = \langle u_{12}(r) | U(r, R) \rangle$  is produced, suitable for zero-range two-nucleon transfer calculations.

$BE \rightarrow EPS$  , the threshold percentage to define components with square norms sufficiently small to be omitted in the final two-nucleon state.

ISC: If  $ISC \leq 0$ , use Gaussian quadrature grid, in blocks of 6th-order positions, for the N-N distance RMIN to RNN ( Card 1).

If  $ISC \geq 1$ , use uniform grid for the N-N distances. Not so accurate.

If  $ISC \neq 0$ , print out numerical values of resulting two-nucleon wavefunction  $U(r, R)$ .

IPC controls the details printed (along with ISC as just above).

$IPC \geq 0$  : one-line summary of  $U(r, R)$  form factor for each  $r$ .

$\geq 1$  : overall norm and rms radius of total NN state.

$\geq 2$  : contour plot of the  $L, \ell$  components included.

$\geq 3$  : contour plot of the  $U(r, R) \times$  interaction potential

$NFL < 0$  : to write two-nucleon wave-function  $U(r, R)$  to file number  $\text{abs}(NFL)$ .

$> 0$  : to read a previously-written wave function from file number  $NFL$ . The values of  $NPAIRS, l_{min}, l_{max}, S_{min}$  of the *present* run are ignored. Thus  $NPAIRS$  can be set to zero.

$NPAIRS$  must be less than or equal to the compilation parameter  $MPAIR$ .

Data cards 14 are now read in, to give details of the single-particle wave functions and their amplitudes in the sum of pairs.

```
Card 14      3 (4 I 3,                                F8.4)
              (NT1 (I) , NT2 (I) , NT3 (I) , NT4 (I) , COEF (I) ) , I=1, NPAIRS
```

The sum over  $I$  of  $COEF(I) |(l_1, s_1) j_1, (l_2, s_2) j_2; J_{12}, T\rangle$ ,

for  $(l_1, s_1) j_1$  given by state  $u_1(r_1)$  of  $KN1 = NT1(I) > 0$ ,

and  $(l_2, s_2) j_2$  given by state  $u_2(r_2)$  of  $KN2 = NT2(I) > 0$ ,

is then transformed into the required  $KIND = 6$  format.

The  $(r_1, r_2)$  coordinates become  $(r, R)$  coordinates, where  $r$  = distance between the two nucleons (angular spin  $\ell$ ), and  $R$  = distance from the core to their centre of mass (corresponding angular momentum is  $L_{nn}$ ).

If  $NT3(I) > 0$ , then the wave functions  $u_1(r_1) \times u_2(r_2)$  are further multiplied by  $u_3(r)$  (of  $KN3 = NT3(I)$ ) before coordinate transformations. Only the radial shape of  $KN3$  is used, not any angular momentum numbers.

If  $NT1(I) = -1$ , then an external form factor is read in from Fortran file number  $NT2(I)$ , and processed using the subroutine `EXTERN1`. At present, this routine is written to read triton wave functions from the Grenoble Faddeev calculations, only reading wave functions, *not* the potential  $\times$  wavefunction (so for e.g. stripping, only use prior interactions).

If  $NT1(I) = -2$ , then an external form factor is read in from Fortran file number  $NT2(I)$ , and processed using the subroutine `EXTERN2`. At present, this routine is written to read 3-body wave functions from HH

calculations, reading wave functions, *as well as* the potential  $\times$  wavefunction. The 'vrr' file format is assumed, and the breakup (third) vertex function is ignored.

If  $NT3(I) < 0$ , then the I'th component of the pair summation is simply the product of cluster wave functions  $u_1(r)u_2(R)$  where  $u_2$  may be  $KIND = 0$  or  $1$ .

$NT4(I)$  is not used in this version of FRESCO.

For  $KIND = 6$ , construct components of the form  $L_{nn}, ((\ell, (s_1, s_2)S_{12})j_{12}; J_{12}, T)$  for all different  $L_{nn}$ ,  $\ell$ ,  $S_{12}$  &  $j_{12}$  values permitted within the limits set by  $\ell_{min}$ ,  $\ell_{max}$ ,  $S_{min}$ , and  $S_{max}$  ( $J_{12}$  and  $T$  are fixed) by summing over pairs of single-particle wave functions.

For all  $KINDs$ , the printout also lists  $DZ$  = derived charge of the bound particle (always positive).

$DM$  = derived mass of the bound particle

$K$  = the wave number of the bound state asymptotically

$NORM$ =overall square norm of this bound state. The wave functions of the single-particle bound states are always normalised to unity.

$RMS$ = root-mean-square radius of this bound state

$D_0$  = zero-range stripping strength for transfers from this state

$D$  = asymptotic stripping strength, as used e.g. in sub-Coulomb transfers

## 2.6 Couplings

Cards 15-17:

Now read in sets of cards for each kind of coupling between partitions and/or between excited states, ending with a card 18 which has ICTO=0. Note that if deformed potentials were given as channel optical potentials then there will already be some couplings between excited states.

Card 15

```
3I4,          3I2,          2F8.2,  2F4.1      2I4
ICTO, ICFROM, KIND,  IP1, IP2, IP3,  P1, P2,  JMAX, RMX,  IP4, IP5
```

The coupling is from all the states in partition ICFROM to all the states in partition ICTO.

Couplings in the reverse direction are also included unless ICTO < 0, except for KINDs 1 & 2 where finer control is allowed.

Couplings are only active for J < JMAX and Radius < RMX, (if JMAX=0, use JTMAX, and if RMX=0, use RMATCH from card 1).

The couplings can be of 8 KINDs:

- = 1 : general spin transfer for projectile/transfer couplings
- = 2 : electromagnetic one-photon couplings
- = 3 : single-particle excitation of the projectile
- = 4 : single-particle excitation of the target
- = 5 : zero-range or LEA transfer with strength P1 and finite range radius P2 (in fm.)
- = 6 : LEA transfer using  $D_0$ . &  $D$  from bound states
- = 7 : finite-range transfer
- = 8 : non-orthogonality correction to a KIND 5,6,7 transfer
- = 9 : same as KIND=1
- =10 : same as KIND=2

After cards 15 for KINDs 2,3,4,5,6,7 (& 8 if IP2>0), spectroscopic amplitudes are read in by means of cards 17. These coupling types are those for which ICTO & ICFROM are different, one being a core partition and the other a composite nucleus. One table is used for all the amplitudes: it is indexed (besides the partition numbers) by IN,IB,IA & KN (see glossary), and stores a real number A. The table is filled cumulatively, starting perhaps with cards 13, so amplitudes need only be entered after the card for the first KIND of coupling in which they appear. (So if all the amplitudes are already entered for a certain KIND of coupling, then the following card 17 will be blank, to indicate no more cards 17 are to be read).

KIND = 1 : General Spin Transfer (with local or non-local external form factors on FILE 4) See Appendix V for more details.

IP1 = 0 : local form factor

1 : non-local (two-dimensional) form factor

IP2 = 0 : read in real values (only if IP3 ≥ 0)

1 : read in imaginary values (only if IP3 ≥ 0)

2 : read in complex values (only if IP3 ≥ 0)

IP3 =3 : read data from JLM folding program jlmP, for projectile couplings only

2 : read data from JLM folding program jlmP, for target couplings only

1 : read data from charge exchange program CHEX2, with appropriate scaling.

0 : no jlmP or CHEX2 scaling factors, only P1, P2 and FSCALE

-1 : write out typical non-local grid ( $R, R'$ ) coordinates

-2 : calculate non-local grid ( $R, R'$ ) coordinates, and call subroutine FFNL to calculate form factor.

-3 : calculate non-local grid ( $R, R'$ ) coordinates, call subroutine FNLSET to calculate an initial form factor, and the call FNLCC for each pair of coupled partial waves, for L-dependent factors.

P1,P2 : scaling for the real and imaginary parts (respectively).

If  $IP3 \geq 0$ , read FROM FILE 4 the following cards (until a blank card):

```
Card 16.6: I4, 3F8.4,           I4, 2F4.0, 2I4, A35
           NP ,HNP,RFS,FSCALE, LTR, PTR,TTR, IB,IA, COMMENT
           for NP = number of radial points
           HNP = step size
           RFS = radius of first point
           FSCALE = scaling factor to be applied
           LTR = L-transfer
           PTR = projectile spin transfer
           TTR = target spin transfer
           IB = excited-state pair fed by coupling
           IA = excited-state pair feeding the coupling
           COMMENT = comment for display in printout.
```

then free format, repeatedly until sufficient data is read.

If  $IP1 = 0$ , read local form factor from  $i=1$  to  $N$

1, read successively for  $j=1, NLO$  the non-local form factors  $FNL(i,j)$ ,  $i=1$  to  $NP$  [ $NLO = RNL / \max(HNL, HCM)$ ]

When  $IP3=1$  for CHEX2 input, the RFS and its F8.4 is omitted from Card 16.6, with default value  $RFS=HNP$ .

$KIND = 2$  : Electromagnetic one-photon couplings (for  $E\lambda$  and  $M\lambda$  processes).

ICTO is the gamma partition and ICFROM the particle partition. The photon must be on the 'projectile' side, and the bound state between target states.

$IP1 = \lambda$  : The multipolarity of the radiation. If  $\lambda > 0$ , include all multipoles  $1, \dots, \lambda$  permitted by parity, whereas if  $IP1 < 0$ , include only the multipole  $\lambda = \text{abs}(IP1)$ .

$IP2 = 0$  : Calculates both electric and magnetic convection couplings

1 : for electric only

2 : for magnetic only

$IP3$ : *not implemented yet*

$KIND = 3$  or  $4$  : Single-particle excitations of the projectile (3) or target (4)

For these KINDs, ICTO is the partition of the nuclei being excited, and ICFROM is used to indicate the *core* partition if the single particle were removed. No couplings are generated to or from the ICFROM partition, only within ICTO partition.

$IP1 = Q$  : The multipole order of the deforming potential due to the colliding nucleus. If  $Q > 0$ , include all multipoles  $0, 1, \dots, Q$  permitted by parity, whereas if  $IP1 < 0$ , include only the multipole  $Q = \text{abs}(IP1)$ .

$IP2$

= 0 : Coulomb & nuclear (complex)



= 1 : nuclear (complex) only  
 = 2 : Coulomb only

IP3

= 0 or 10 : include all re-orientation terms  
 = 1 or 11 : no re-orientation terms for  $Q > 0$   
 = 2 or 12 : ONLY re-orientation terms  
 = 3 or 13 : include only couplings to and from the ground state, but NOT gs reorientation,  
 = 4 or 14 : include diagonal couplings, and couplings to and from the ground state  
 = 5 or 15 : include diagonal couplings, and couplings to and from any bound state  
 $\geq 10$  : read cards 16.5, repeating FORMAT(6E12.4) as required, for complex factors  
 QSCALE(Q),  $Q = \max(0, -IP1)$ ,  $\text{abs}(IP1)$  to scale the folded form factors for multipoles Q.

IP4 =  $Q_{\max}$ , the max deformed core potential multipole

IP5 =  $\Lambda_{\max}$ , the new multipole order for formfactor reduction (see Appendix III).

P1 = FLOAT( potential KP index for fragment - target interaction)

P2 = FLOAT( potential KP index for core - target interaction)

(only SCALAR parts of the potentials P1 and P2 are used).

KIND = 5 or 6 : Zero-range & LEA transfers for projectiles

IP1 and IP2 not used.

For KIND=5,

P1 =  $D_0$  - ZR coupling constant

P2 = FNRNG - Effective finite-range parameter for use in LEA (in units of fm.)

For KIND=6, use  $D_0$  and  $FNRNG = \sqrt{(D/D_0 - 1)/k^2}$ . from the projectile bound states. With unbound states,  
 or if IP3 = 1, use  $D_0$  from state, but FNRNG = P2 from input card here.

In both KINDs, read in cards 17, noting that for KIND = 5 spectroscopic factors for the projectile are not needed, and are ignored.

Users of these interactions kinds should also pay attention to the PARAMETER INH as described in Appendix I.

KIND = 7 : Finite-range transfers.

IP1 = 0,-2 : POST interaction

1,-1 : PRIOR interaction (N.B. meaning of IP1 thus depends on ICTO & ICFROM!!!)

$\leq -1$  : Use  $\theta$  quadrature from  $\theta = \pi$  down to  $\theta = 0$ . (Useful for finite-range knock-on with light projectiles)

$\leq -3$  : 'VCORE' interaction: Use ONLY the core-core interaction potential (Useful for finite-range knock-on with light projectiles)

IP2 = 0 : no remnant

1 : full real remnant

-1 : full complex remnant

2 : "non-orthogonality remnant" - this works by inserting a KIND = 8 coupling card after this coupling, before any subsequent couplings. This is does not affect the one-step amplitudes, and is only useful if another transfer step follows this coupling.

IP3 = KPCORE : the number KP of the potential to use between the two cores, in the remnant part of the interaction potential.

If IP3=0, use as KPCORE the optical potential given for the first pair of excited states in the partition of projectile core. (this uses the observation that optical potentials tend to depend more on the projectile than the target, and must clearly be re-examined if the projectile is heavier than the target.)

P1,P2 : not used.

KIND = 8 : Non-orthogonality supplement appropriate to a previous KIND 5,6 or 7 interaction.

IP1 = 0 : post

1 : prior (N.B. IP1 should be the same as the previous interaction!)

IP2

> 0 : read in spectroscopic factors as cards 17 (Only useful if you did NOT have a previous KIND 5,6,7 interaction, which would have needed the amplitudes then.)

= 0 : no cards 17 to read.

Note that you should *either* use KIND=7, |IP2|=2, *or* use KIND=7, |IP2|=1 and a KIND=8. If you have KIND=7, |IP2|=2 and a KIND=8 card, then this is double counting.

Cards 17:

*Spectroscopic amplitudes* for the overlaps between partitions ICTO & ICFROM already defined by a card 15.

Read until IN = 0 or IN < 0:

4X, 4I4, F8.4

IN, IB, IA, KN, A

meaning that the overlap of the composite nucleus in excitation state IB with the core nucleus in excitation state IA is the bound-state form factor KN with amplitude A. The IN=1 specifies projectile overlap, and IN=2 target overlap.

If the form factor KN mixes different IA levels, then the spectroscopic amplitudes should rather be specified with a Card 13.

N.B. The amplitudes A are signed, and are NOT the spectroscopic factors, but will typically be the square roots of these factors. For transfers out of or into closed shells of N antisymmetrised nucleons, the spectroscopic factors will usually contain factors of N, so the spectroscopic amplitudes needed by FRESCO will typically need to already contain factors of  $\sqrt{N}$ .

The sign of A should be consistent with the spin coupling order used in the program, which is

$$(\ell, s)j, J_{core}; J_{com}$$

for binding a  $\ell s j$  nucleon onto a core of spin  $J_{core}$  to form  $J_{com}$ .

If IN<0, use abs(IN) in this the last card 17

If IN=0, no more cards 17 to be read.

## 2.7 Incoming Channel, Energy

Card 18: (has the first 4 columns blank or zero : ie card 15 with ICTO=0)

3I4, 3I2

0, PEL, EXL, LAB, LIN, LEX

Incoming plane waves are present in partition PEL with excitation pair EXL. The energies on card 19 are the laboratory energies for partition LAB's nucleus LIN (1 or 2 for projectile or target) in excitation pair LEX.

The defaults for PEL, EXL, LIN & LEX are all 1, and the default for LAB is PEL, so this card can be completely blank usually.

Card 19 : Projectile Energies

3(F8.4,I8),F8.4) : (ELAB(i),NLAB(i),i=1,3),ELAB(4)

A series of runs at different (real) energies until ELAB(i) = 0 is found. If NLAB(i) > 1, then the range from ELAB(i) to ELAB(i+1) is covered in NLAB(i) linear intervals.

## 2.8 Additional Cards on Fortran input file 4:

All these cards involve reading real or complex floating point numbers by repeating

FORMAT(6E12.4)

Cards A1 : External Potential Form Factors (SHAPEs 7-9 on Cards 10)

Cards A2 : External Coupling Potentials for KIND 1 & 2 couplings (NO < 0 on Cards 16)

## Appendix I : FRESCO Namelist input in Fortran 90 version

This Fortran 90 version does dynamic allocation of arrays of the required sizes, and therefore does not need the PARAMETER declarations which were a feature of previous FRESCO input specifications. The FRESCO executable can be now completely compiled in advance, and does not require other files (such as, previously, frxp0.f and libfrxp.a) to run.

The f90 version reads card sequences as above, but can also read NAMELIST input, which is more flexible in allowable number formats.

After the usual Card 0 with title information, the line

```
Card 1:  
NAMELIST
```

indicates namelist input is to be assumed. A namelist group starts with a &NAME and ends with a /. Upper and lower case names are treated as equivalent. For a sample input, see Appendix II.

If Card 1 begins with 'CDCC', then CDCC input is assumed, see Appendix III.

The first namelist read is &FRESCO ... /:

### &FRESCO namelist

This contains all the variables in Cards 1,1a, 2, 3, 4, 5 and 18 and 19:

```
hcm, rmatch, rintp, hnl, rnl, centre, rasy, accrcy, switch, ajswtch,  
jtmin, jtmax, absend, dry, rela, nearfa,  
kqmax, pp, thmin, thmax, thinc, koords, cutl, cutr, cutc,  
ips, it0, iter, iblock, pade, iso, nnu, maxl, minl, mtmin, epc,  
inh, plane, smallchan, smallcoup,  
chans, listcc, treneg, cdetr, smats, xstabl, nlpl, waves, lampl, kfus, wdisk,  
pel, exl, lab, lin, lex, elab, nlab
```

along with new variables

```
fatal, nosol, pset, jset, inh, psiren, tmp, masfil, unitmass, finec.
```

The new variables are:

fatal = T/F, if to stop or not when CRC iterations do not converge (previously ITER>0).

nosol = T/F, if not to solve the CRC equations, only construct couplings (previously —ITER—<IT0).

pset = -1 or +1, to restrict parity of total CRC set (0 = no restriction) (previously from CSET).

jset = number of CRC sets to calculate before stopping (0 = all sets) (previously from CSET).

inh = 0 : zero-range transfer forms in intervals of HCM exactly (previously a PARAMETER).

    = 1 : stored in steps of HCM \* (proj. core)/(proj. composite mass)

    = 2 : stored in steps of HCM \* (targ. core)/(targ. composite mass)

    So inh=2 corrects for longitudinal recoil during transfers with zero-range projectiles.

psiren = T/F, to do simple renormalisation of channel wfs after Pade acceleration

tmp = name of directory for temporary files: '/tmp' or '.'

masfil = name of file of masses of isotopes (used to find masses and charges from the nuclide name, if read-in MASSes are zero).

unitmass = unit (in amu) for MASS values read in. Default = 1.000

finec = fine-structure constant: used to determine electrostatic  $e^2$ . Default = 137.03599d0.

jump, jbord = namelist input jump(1) is stored in jump(2) etc for the program.

### **&PARTITION namelist**

This has the information on Card 6, but the names have been made unique:

namep	massp	zp	nex	pwf	namet	masst	zt	qval
(char*8	real	real	int	logical	char*8	real	real	real)

### **&STATES namelist** Card 7 information: repeat NEX times before the next partition namelist:

```
Jp, COPYp,BANDp ,Ep, KKp,Tp, CPOT,PWF,  
-----projectile state-----
```

```
Jt, COPYt,BANDt ,Et, KKt,Tt, EXTRA,SPIFL,IGNORE  
-----target state-----
```

Here, PTYp and PTYt are synonyms for BANDp and BANDt, respectively.  
KP has been renamed CPOT, and the band-head projections are KK\*.

End reading partitions with an empty namelist &partition / (Card 8)

**&POT namelist** This has the information on Cards 9 and 10. You can either input individual &pot namelists corresponding to each separate Card 9 and Card 10, or you can combine TYPEs 0,1,2,3, 10 and 11 potentials into a larger namelist.

**Individual namelists:** Variables kp, type, shape, itt, p(1:7), where itt is a logical variable. The p(1:7) is synonymous to the set p1, p2, p3, p4, p5, p6, p7, and with the array def(:). The equivalent to Card 9 is obtained if shape=0, then A#1=p1, A#2=p2, R0C=p3, and AC=p4.

**Combined namelists:** All the following variables may be set independently in the &pot namelist

```
kp      shape itt  
ap      at      rc      ac  
v        rv      av      w      rw      aw  
wd      wdr      wda      vd      vdr      vda  
vso      rso      aso      vsoi rsoi asoi  
defp(:)  deft(:)  mnet(:)  mnep(:)=0
```

so A#1=at,A#2=ap, R0C=rc, and AC=ac etc. All the potentials will have the same shape.

The mnep(k) and mnet(k) are the TYPE=11 and 12 Coulomb reduced matrix elements, and the defp(k) and deft(k) are the TYPE=11 and 12 nuclear deformation lengths. matrix elements, for multipolarity k. This combined namelist is a pre-processing option only: the FRESCO output will be the same as from individual namelists.

More complicated potentials may be formed as usual by having multiple &pot namelists, but keep only **one** Coulomb potential by having rc non-zero in only **one** of them.

End reading potentials with an empty namelist &pot / (Card 12), or by having kp<0 in the last namelist.

**&STEP namelist** The information on Card 11 is give by a `&step` namelist with variables `IB, IA, k, STR`.

**&OVERLAP namelist** This namelist has the standard variables of Card 13 `kn1, kn2, ic1, ic2, in, kind, ch1, nn, l, lmax, sn, ia, j, ib, kbpot, krpot, be, isc, ipc, nfl, nam, ampl` with the same names.

Extra variables `keep, dm, nk, er, e` are also defined:

`keep = T` to **not** reset all the variables to zero before reading next namelist.

`dm` = mass of bound particle, if to override default difference.

`nk` = number of integration steps to form continuum bin.

`er` = range (width) of continuum bin. If `er > 0`, then **ratio** of the upper and lower bin energies; and if `er < 0`, then `er` is the **difference** of the energies in MeV.

`e` : If `e ≠ 0`, then replace `be`  $\leftarrow -e$ .

So `be` = binding energy, and `e` = eigenenergy.

### **&COUPLING namelist**

This gives the information previously on Card 15.

`icto, icfrom, kind, ip1, ip2, ip3, p1, p2, jmax, rmax, kfrag, kcore`  
`int int int int int int 4*real int int`

If(`kfrag`>0) `p1`  $\leftarrow$  `kfrag`, and if(`kcore`>0) `p2`  $\leftarrow$  `kcore`.

**&INEL namelist** The information on Card 16 is give by a `&inel` namelist with variables `ib, ia, k, no, kp, a`.

**&CFP namelist** The information on Card 17 is give by a `&cfp` namelist with variables `in, ib, ia, kn, a, keep`.

**&SCALE namelist** The information for Coupling KINDS 3 and 4 is given by a `&scale` namelist with variables `QSCALE(0:11)`.

## **Mass and charge constants**

To exactly reproduce previous FRESCO runs using  $2 * amu / \hbar^2 = 0.0481960$ , you will need to enter to this version the numbers: `unitmass=1.007335d0; finec=137.5648d0`. To exactly reproduce using  $2 * amu / \hbar^2 = 0.0478326$ , you need input `unitmass=0.999740d0; finec=137.0455d0`, but only the default input of `unitmass=1d0; finec=137.03599d0` is completely accurate.

## **Glossary of Indexing Variables**

`IC, IC1, IC2` index to mass partitions

`IA, IB` index to projectile-target pairs of excited states within each partition

`KP` index to table of potentials, for scattering, binding, and folding

`KN` index to single-particle bound states

`KN1, KN2` two-particle bound states are given for a range (`RMIN` to `RNN`) of internucleon separations, and are stored in the MSP table from `KN1` to `KN2` inclusive.

`CP` index to the coupling set up

## Appendix II : A Test Run (a CCBA calculation)

The following test case calculates the inelastic and transfer cross sections for the reactions induced by  $^{19}\text{F}$  on  $^{28}\text{Si}$  at 60.0 MeV. A Triton-Oxygen cluster structure is assumed for  $^{19}\text{F}$ , with the potentials for the triton and the oxygen core being folded together to give a diagonal Watanabe potential for elastic  $^{19}\text{F}$  scattering as well as the couplings to the inelastic  $1/2+$  state. These elastic and inelastic channels are coupled together to all orders, then a finite-range transfer step is calculated for the  $^{16}\text{O} + ^{31}\text{P}$  channel, thus performing a CCBA calculation. The Card types and line numbers added here only for convenience:

```

0  04 Test run: CCBA calculation 28Si(19F,16O) 31P, cluster form factors.
1  05 0.10      25.0    0.50    0.100    3.
2  06  0. 80.    .01    F F
3  07 1 0.0     60.0    2.5
4  08 0.00      1 2 0 30      0 0.0
5  09 1 2 0 0 1 0 0 0 0 0
6  10 19-F      19.0    9.0      2 28-SI    28.0    14.0    0.0
7  11 0.5      +1 0.0      0      0.0      +1 0.0
7  12 2.5      +1 0.2
6  13 16-O      16.0    8.0      1 31-P      31.0    15.0    6.199
7  14 0.0      +1 0.0      0      0.5      +1 0.0
8  15
9  16  1 0  0 28.0      19.0    1.2
9  17  2 0  0 31.0      16.0    1.35
10 18  2 1  0 31.20    1.45    0.47    15.10    1.270    0.310
10 19  2 3  0  0.75    1.24    0.37
9  20  3 0  0 19.0     0.0      1.25     0.65
10 21  3 1  0 115.00   1.250    0.650
10 22  3 3  0  6.30    1.25    0.650
9  23  4 0  0 31.0     0.0      1.25     0.65
10 24  4 1  0 99.000   1.250    0.650
10 25  4 3  0  6.30    1.25    0.650
9  26  5 0  0 28.0     0.0      1.2
10 27  5 1  0 27.00    2.42452  0.460    11.66    2.14456  0.238
9  28  6 0  0 28.0     0.0      1.25     0.65
10 29  6 1  0 160.00   1.07    0.72    37.0     1.35     0.88
10 30  6 3  0  10.0    0.85    0.850
12 31 0
13 32  1      1 2 1 0    4 0    0.5    0.5    3 0    11.73    1 0 0
13 33  2      1 2 2 0    4 0    0.5    0.5    4 0    17.899    1 0 0
13 34  3      1 2 1 0    3 2    0.5    2.5    3 0    11.53    1 0 0
13 35 0
15 36  2      1      7 0 0 0
16 37      1      1  1  1  1.00
16 38      1      2  1  3  1.00
16 39      -2      1  1  2  1.00
15 40  1      2      3 4 1 0  6.0      5.0
16 41
18 42  0      1      1
19 43 60.0

```

A namelist version of the above input is:

Test run: CCBA calculation 28Si(19F,16O) 31P, cluster form factors.

NAMELIST

&FRESCO

hcm=.10 rmatch=25 rintp=0.50 hnl=0.100 rnl=3.  
jtmin=0. jtmax=80 absend=.01 kqmax=1 thmin=0. thmax=60.0 thinc=2.5  
iter=1 iblock=2 nnu=30 chans=1 listcc=2 smats=1 elab=60.0  
/

&PARTITION

namep='19-F' massp=19. zp=9 nex=2 namet='28-SI' masst=28 zt=14 /  
&states Jp=0.5 Bandp=+1 Ep=0.0 cpot=1 Jt=0.0 bandt=+1 Et=0.0 /  
&states Jp=2.5 Bandp=+1 Ep=0.2 /

&PARTITION

namep='16-O' massp=16. zp=8 nex=1 namet='31-P' masst=31 zt=15 qval=6.199/  
&states Jp=0.0 Bandp=+1 Ep=0.0 cpot=2 Jt=0.5 bandt=+1 Et=0.0 /  
&partition /

&pot kp=1 At=28.0 Ap=19.0 Rc=1.2 /  
&pot kp=2 At=31.0 Ap=16.0 Rc=1.35  
V=31.20 rv=1.45 av=0.47 W=15.10 rw=1.270 aw=0.310  
Vso=0.75 rso=1.24 aso=0.37 /  
&pot kp=3 At=19.0 Rc=1.25 ac=0.65  
V=115.00 rv=1.250 av=0.650 Vso=6.30 rso=1.25 aso=0.650 /  
&pot kp=4 At=31.0 Rc=1.25 ac=0.65 V=99.000 rv=1.250 av=0.650  
Vso=6.30 rso=1.25 aso=0.650 /  
&pot kp=5 At=28.0 Rc=1.2  
V=27.00 rv=2.42452 av=0.460 W=11.66 rw=2.14456 aw=0.238 /  
&pot kp=6 At=28.0 Rc=1.25 ac=0.65  
V=160.00 rv=1.07 av=0.72 W=37.0 rw=1.35 aw=0.88  
Vso=10.0 rso=0.85 aso=0.850 /  
&pot /

&OVERLAP kn1=1 ic1=1 ic2=2 in=1 kind=0 nn=4 l=0 sn=.5 j=0.5 kbpot=3 be=11.73 isc=1 /  
&OVERLAP kn1=2 ic1=1 ic2=2 in=2 kind=0 nn=4 l=0 sn=.5 j=0.5 kbpot=4 be=17.899 isc=1 /  
&OVERLAP kn1=3 ic1=1 ic2=2 in=1 kind=0 nn=3 l=2 sn=.5 j=2.5 kbpot=3 be=11.53 isc=1 /  
&overlap /

&COUPLING icto=2 icfrom=1 kind=7 ip1=0 ip2=0 ip3=0/  
&cfp in=1 ib=1 ia=1 kn=1 a=1.00 /  
&cfp in=1 ib=2 ia=1 kn=3 a=1.00 /  
&cfp in=2 ib=1 ia=1 kn=2 a=1.00 /  
&cfp /

&COUPLING icto=1 icfrom=2 kind=3 ip1=4 ip2=1 ip3=0 kfrag=6 kcore=5/



## Appendix III : CDCC Namelist input in Fortran 90 version

### &CDCC namelist

hcm, rmatch, rintp, hnl, rnl, centre, rsp, iter, pset, llmax, dry, rasym, accrcy, switch, ajswtch, sinjmax, cutl, cutr, cutc, absend, jtmin, jump, jbord, nnu, rmatr, nrbases, nrbmin, pralpha, pcon, meigs, listcc, smats, veff, chans, xstabl, thmin, thmax, thinc, smallchan, smallcoup, melfil, nosol, cdetr, numnode, treneg, nlpl, trans, pel, exl, cdccc, qscale, pade, kfus, elab, lab, lin, lex,

hktarg, ncoul, reor, pauli, nk, q, ipc, iscg, ipcg, hat, remnant, postprior, quasi, sumform, qc, la, static, expand, maxcoup

are all the same as the **&FRESCO** namelist, except for:

- cdccc which is an alias for cdcc of Card 5,
- q = ip1, multiple for the projectile single-particle couplings,
- ncoul = ip2, selecting nuclear and/or coulomb,
- reor = ip3, selecting diagonal and/or off-diagonal couplings,
- qc = ip4,  $Q_{\max}$  for the deformed core potential multipoles,
- la = ip5,  $\Lambda_{\max}$  for the new multipole orders with formfactor reduction,
- hat (logical, default T) to use mean bin energies (otherwise midpoint),
- quasi: if assigned, set all channel energies as if for this projectile energy (eg -be for adiabatic),
- iscg, ipcg = isc, ipc (card 13) for the projectile ground state wave function,
- elab = ELAB (1), just the one projectile lab energy,
- hktarg = target value of  $h.K$ , where  $h=HCM$  and  $K$  is the elastic wave number. (default hktarg=0.2).  
If HCM=0 on Card 1, then  $h$  is calculated from elab and hktarg.

sumform determines the bin formfactor reductions (default 2 if there are any kind=3 bin states, else 0):

- = 0 : no formfactor reduction:  $\langle KN|KQ\lambda|KNP \rangle$
- = 1 :  $KQ\lambda$  formfactors summed into new multipole  $\Lambda$ :  $\langle KN|\Lambda|KNP \rangle$
- = 2 : formfactors summed into composite projectile state:  $\langle IB|\Lambda|IBP \rangle$ . This is not allowed if have spin-orbit or transfer couplings, and sumform=1 will be set in these cases.

If have no cc bins, then  $K$  multipoles truncated using ip1=q.

If have cc bins and  $Q_{\max}=qc=ip4$  and  $\Lambda_{\max}=la=ip5$  are unset, then q sets the maximum multipole order of  $\Lambda$ , and all possible values of  $KQ\lambda$  are used that couple to  $\Lambda \leq q$

If qc and la are both set, then control each multipole individually:

- q =  $K_{\max}$ , ip1 set in usual way
- ip4=qc =  $Q_{\max}$ .
- ip5=la =  $\Lambda_{\max}$  maximum order for new multipole.
- Note:  $\lambda$  will always run from  $0 \rightarrow Q$ .

trans determines the number of transfer partitions:

- = 0 : no transfers: no E(jectile) or R(esidue)
- < 0 : only R(esidue): the Ejectile and Core are identical
- > 0 : both E(jectile) and R(esidue) independently of Core nucleus.

postprior = ip1 for finite-range transfer couplings,

remnant = ip2 for finite-range transfer couplings,

pauli = attempted Pauli blocking using non-orthogonality couplings.

### &NUCLEUS namelist

part, name, mass, charge, spin, parity, be, n, l, j, ia, a, kind, lmax, nch, nce, ampl

where this card is repeated for each part beginning P: projectile, C: core, V: valence, T: target, E: ejectile, R: residue.

The number of nuclei (4, 5 or 6) depends on trans: see above.

name, mass, charge as name, mass, zp/t on Card 6,

spin, parity as Jp/t, Bandp/t on Card 7.

be, n, l, j, ia, a, kind, lmax, nch prescribe the projectile P bound state, and with transfers also for residue R. nce is the number of Core excited states.

If nce>0, then read that number of **&CORESTATES** namelists.

**&CORESTATES namelist:** spin, parity, ex

for spin, parity ( $\pm 1$ ) and excitation energy of each Core state above the ground state.

#### **&BIN namelist**

spin, parity, step, start, end, energy, n, l, j, isc, ipc, kind, lmax, nch, ia, il, ampl

These are repeated until an empty **&BIN** namelist is encountered (step=0).

Each bin set has the same spin, parity, l, j, isc, ipc, kind, lmax, nch, ia, il, ampl, but a different energy. The energy range is divided into (end-start)/step bins. If energy then these are evenly spaced in energy, else they are evenly spaced in momentum  $k \propto \sqrt{E}$ . Changing or starting partial waves is equivalent to start=0.001.

The values of lmax, nch, ia, il are only needed coupled channels bins kind=3, with il being the channel number of the incoming partial wave, which, if il=0, is defined as the channel with quantum numbers l, j and ia. The array ampl gives overall multiplicative spectroscopic amplitudes to the bin. The values of isc, ipc, kind, lmax have the same meaning as in Card 13, with j an alias for jn.

If l, j, ia are not set then kind=3 coupled-channels bins are generated using lmax, for all incoming waves. Setting il will select an incoming channel.

#### **&POTENTIAL namelist**

part, a1, a2, rc, ac, v, vr0, a, w, wr0, aw, wd, wdr0, awd, vso, rso0, aso, shape, freal, fimag, vsot, rsot0, asot, l, parity, nosub, itt, beta2, beta3, ideo, beta2c, beta3c, beta2m, beta3m

where this card is repeated for each part beginning P: projectile-target optical potential, C: core-target optical potential, V: valence-target optical potential, T: projectile (C+V) ground state, B: projectile channels *not* containing the ground state, T: transfer channel optical potential, E: ejectile bound state, R: residue bound state.

Different part=B(in) potentials may be defined depending on parity or partial wave l.

nosub means that the P(projectile) optical potential is *added* to the CDCC couplings as a diagonal in all projectile state channels.

For deformations, beta2m, beta3m are the nuclear *fractional* deformations, and beta2c, beta3c are the Coulomb equivalents (both with default values beta2, beta3 respectively).

The Coulomb and nuclear deformations may also be restricted by ideo:

= 0 : Coulomb & nuclear (complex)

= 1 : nuclear (complex) only

= 2 : Coulomb only

### Sample CDCC input file:

```
11Be+4He spdf; 1+5*10+2*5 chs 0-10 MeV, q=0-3 2200 MeV, 30/100 fm
CDCC
&CDCC
  hcm=0 rmatch=-30 absend=-50 rasym=100 accrcy=0.001
  elab=2200
  jbord= 0 60 200 2500
  jump = 4 5 20
  thmax=30 thinc=.05 smats=2 xstabl=1 cutr=-10 cutc=0
  nk=50 ncoul=0 reor=0 q=3
/
&NUCLEUS part='Proj' name='11Be' spin=0.5 parity=+1 be = 0.500 n=2 l=0 j=0.5 /
&NUCLEUS part='Core' name='10Be' charge=4 mass=10 /
&NUCLEUS part='Valence' name='neutron' charge=0 mass=1 spin=0.5/
&NUCLEUS part='Target' name='4He' charge=2 mass=4 /

&BIN spin=0.5 parity=+1 step=0.5 end=10. energy=F l=0 j=0.5/
&BIN spin=0.5 parity=-1 step=0.5 end=10. energy=F l=1 j=0.5/
&BIN spin=1.5 parity=-1 step=0.5 end=10. energy=F l=1 j=1.5/
&BIN spin=1.5 parity=+1 step=1.0 end=10. energy=F l=2 j=1.5/
&BIN spin=2.5 parity=+1 step=1.0 end=10. energy=F l=2 j=2.5/
&BIN spin=2.5 parity=-1 step=2.0 end=10. energy=F l=3 j=2.5/
&BIN spin=3.5 parity=-1 step=2.0 end=10. energy=F l=3 j=3.5/
&BIN /

&POTENTIAL part='Proj' a1=11 a2=4 rc=1.0 /
&POTENTIAL part='Core' a1=10 a2=4 rc=1.0
  V=46.92 vr0=1.204 a=0.53 W=23.46 wr0=1.328 aw=0.53 /
&POTENTIAL part='Valence' a1=4 rc=1.3
  V=37.14 vr0=1.17 a=0.75 W=8.12 wr0=1.26 aw=0.58 /
&POTENTIAL part='Gs' a1=10 v=51.51 vr0=1.39 a=.52 vso=0.38 rso0=1.39 aso=0.52/
&POTENTIAL part='Bi' a1=10 v=28.38 vr0=1.39 a=.52 vso=0.38 rso0=1.39 aso=0.52/
```

## Appendix IV : FORTRAN file allocations

File no.	Format (Fix/Var)	LRECL (bytes)	Access (Seq/Ran)	Routines	Use
1	V		S	SFRESKO	FRESKO input when searching
2	V		S	SFRESKO	Search specification file
3	V		S	FREADF, FR	Temporary namelists file
4	F	80	S	INTER POTENT	external KIND=1,2 form factors external potentials
5	F	80	S		standard input
6	V	142	S		standard output
7	F	80	S	DISPX	elastic S-matrix elements
8	F	sector	R	FR,INTER	s/p wfs, channel wfs
9	F	NLL*NLO*16	R	Q/KERNEL	complex transfer multipoles
10	V		S	FR,CRISS	S-matrix elements (cfs)
11	F	NLL*NLO*8	R	Q/KERNEL	real transfer multipole
12	V	NLL*NLO*16	S	KERNEL/SOURCE	transfer kernels
13	F	80	S	FR	total cross sections for each Elab
14	V		S	INTER/CPAIR	interaction potentials
16	F	80	S	CRISS	tables of cross sections
17	F	80	S	FR	output scattering waves
18	V		S	FR	wfns of 'best' iterate
19	F	N	S	FR	Local couplings
20-33				Available for users	(eg bound states, amplitudes)
34	F	80	S	POTENT	output potentials
35	F	80	S	FR	Astrophysical S-factors for Ecm
36				CRISS	output scattering AMPL amplitudes
37				CRISS	output scattering FAM amplitudes
38	F	80	S	DISPX	cross sections for each J/pi
39	F	80	S	FR	2 cross sections for each Elab
40	F	80	S	FR	all cross sections for each Elab
41	F	80	S	SOURCE	source terms at each iteration
42	F	80	S	SOURCE	bin wavefunctions for each E
43	F	80	S	INFORM	bin phase shifts as k functions
44	F	80	S	INFORM	bin phase shifts as E functions
45	F	80	S	ERWIN	scat phase shift as E functions
46	F	80	S	INFORM	bs wave functions & Whit ratios
47	F	80	S		reduced matrix elements
48	V	133	S	FR	misc log file
55	F			INFORM	Single-particle wave functions
56	F			FR	Jtotal fusion & reaction cross
57	F			FR	Output of CDCC amplitudes
58	F			INFORM	Bound state wave functions
59	F			INFORM	Bound state vertex functions
60-62	F			RMATRIX	Trace of R-matrix calculations
66	V	NLL*NLO*16	S	INTER	KIND=1 nonlocal formfactor
71	F	132	S	FR	20 pw phase shifts as Elab functions
75	F		S	FR	Astrophysical S-factors for Elab
89	F			MULTIP	Folded coupling potentials

File no.	Format (Fix/Var)	LRECL (bytes)	Access (Seq/Ran)	Routines	Use
105	V		S	FCN	$\chi^2$ progress during fitting
200	F	80	S	CRISS	Elastic cross section if not fort.201
201-210	F	80	S	CRISS	Cross sections (cf 14) for states 1-10
301	V		S	CDCIN	New Fresco input
302	V		S	CDCIN	New Fresco input (temp)
303	V		S	SFRESKO	Input search file
304	V		S	SFRESKO	Output plot file
305	V		S	CDCIN	New Fresco input from cdcin, col format
306	V		S	SFRESKO/FRXX0	Input Fresco file
307	V		S	SFRESKO/FRXX0	Initial Output Fresco file
308	V		S	SFRESKO/FRXX0	Main Output Fresco file

## Appendix V : KIND=1 Spin Transfer Couplings

The definition of the KIND=1 spin transfer couplings is not given in the Computer Physics Reports article, so in versions after March 1998 these are redefined for IP3=0 or 1, and new Racah algebra factors included.

We want to calculate the coupling interactions of the monopole operator  $\mathbf{S}([\ell, s_p]s_t, s_t)$ , where  $s_p$  is the spin transfer of the projectile  $I_p$ ,  $s_t$  is the spin transfer of the target  $I_t$ , and  $\ell$  is the orbital angular momentum transfer. These coupled operators are defined following in Bohr & Mottelson, Vol. 1, section 1A-5c, as

$$(F_{\lambda_1} G_{\lambda_2})_{\lambda\mu} = \sum_{\mu_1 \mu_2} \langle \lambda_1 \mu_1, \lambda_2 \mu_2 | \lambda \mu \rangle F_{\lambda_1 \mu_1} G_{\lambda_2 \mu_2} , \quad (1)$$

applied for the case of  $F_{s_t} = [\ell, s_p]s_t$  and  $G_{s_t} = s_t$ . The overall  $\mathbf{S}$  operator is a monopole (scalar), for which the tensor product is thus of the kind

$$(F_{\lambda} G_{\lambda})_{00} = (2\lambda + 1)^{-1/2} \sum_{\mu} (-1)^{\lambda - \mu} F_{\lambda \mu} G_{\lambda - \mu} . \quad (2)$$

This differs from common definitions (eg of Satchler) by a factor of  $(-1)^{\lambda}(2\lambda + 1)^{-1/2}$ .

Reduced matrix elements are defined everywhere in FRESKO by:

$$\langle j_f m_f | \hat{O}_{\lambda\mu} | j_i m_i \rangle = (2j_f + 1)^{-1/2} \langle j_i m_i, \lambda \mu | j_f m_f \rangle \langle j_f || \hat{O}_{\lambda} || j_i \rangle \quad (3)$$

The matrix elements of this operator are

$$\begin{aligned} & \langle (LI_p)J, I_t; J_T M_T | \mathbf{S}([\ell, s_p]s_t, s_t) | (L'I'_p)J', I'_t; J_T M_T \rangle \\ &= (-1)^{s_t + J_T + J' + I_t} \left\{ \begin{matrix} J' & I'_t & J_T \\ I_t & J & s_t \end{matrix} \right\} \hat{J} \hat{J}' \left\{ \begin{matrix} L' & I'_p & J' \\ \ell & s_p & s_t \\ L & I_p & J' \end{matrix} \right\} \frac{1}{\sqrt{4\pi}} \hat{\ell} \hat{L} \langle L0 \ell 0 | L'0 \rangle \\ & \times \langle I_p || s_p || I'_p \rangle \langle I_t || s_t || I'_t \rangle \end{aligned} \quad (4)$$

In using KIND=1 couplings with IP3=0, the first line of these factors is generated automatically. The product of the reduced matrix elements for the intrinsic nuclear states,  $\langle I_p || s_p || I'_p \rangle \langle I_t || s_t || I'_t \rangle$ , has to be included explicitly in the factor FSCALE, or in the radial form factors. The radial shapes have to be read in using Cards 16.7.

With IP3=2, implying jlmP input for target-only couplings,

- the projectile diagonal reduced matrix element  $\langle I_p || s_p = 0 || I_p \rangle = \hat{I}_p$  is supplied by Fresco,
- the factor  $1/\sqrt{4\pi}$  is omitted above,
- and an additional symmetric factor of  $((2I'_t + 1)(2I_t + 1))^{1/4}$  is supplied to allow the monopole radial form factors to have their physical values for any target spin.
- The forward and reverse form factors should be identical for Hermitian couplings.

With IP3=3, implying a similar input for projectile-only couplings,

- the target diagonal reduced matrix element  $\langle I_t || s_t = 0 || I_t \rangle = \hat{I}_t$  is supplied by Fresco,
- the factor  $1/\sqrt{4\pi}$  is omitted above,
- and an additional symmetric factor of  $((2I'_t + 1)(2I_t + 1))^{1/4}$  is supplied to allow the monopole radial form factors to have their physical values for any target spin. The forward and reverse form factors should be identical for Hermitian couplings.

## Appendix VI : Search version SFRESCO

This is a program which searches for a  $\chi^2$  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.

A `search_file` format is defined as follows:

Card 1:

```
(2*string, 2*integer: free format)
input_file, output_file, nvariables, ndatasets
```

`input_file`: name of file (in single quotes) with regular FRESCO input

`output_file`: name of file for the final FRESCO output

`nvariables`: number of search variables

`ndatasets`: number of experimental data sets.

Repeated `nvariables` times, a namelist with some of the following variables:

```
Card 2: (namelist: 'variable')
name, kind, step, valmin, valmax, null,
kp, pline, col, potential,
dataset, datanorm,
nafrac, afrac,
energy, jtot, par, channel, width
```

`name` is name of variable (up to 10 characters),

`kind`: 0=ignore, 1=potential, 2=afrac, 3=R-matrix energy,  
4=R-mat partial width, 5=dataset normalisation

`step`: step size for finding derivatives etc, zero for fixed. (default 0.01)

`valmin`: strict lower bound (if non-zero),

`valmax`: strict upper bound (if non-zero),

`null`: (default -124578) 'undefined' value,

**kind=1: Variable potential parameter:**

`kp`: number of potential as on Card 10,

`pline`: order of which Card 10 within potential definition,

`col`: number on Card 10: selecting P0–P7 ,

`potential`: value of this potential parameter (default `null`: use `input_file`)

**kind=2: Variable spectroscopic amplitude:**

`nafrac`: order number of Cards 17 in `input_file`

`afrac`: spectroscopic amplitude A (default `null`: use `input_file`)

**kind=3: Variable energy of R-matrix term:**

`term`: term number (default 1)

`jtot`: J value for additional R-matrix term

`par`: parity (+1 or -1)



energy: energy (cm MeV in entrance channel) of additional R-matrix term (default 0)  
nopot: Disable potential & Buttle correction for this J/pi set (logical T or F, default F)

**kind=4: Variable partial width of R-matrix term:**

channel: channel number (in order generated by FRESCO)

term: term number (default 1)

width: width for this channel ( $\text{MeV}^{1/2}$ ) (default 0)

**kind=5: Variable dataset normalisation:**

dataset: index of which dataset (1 up to `ndatasets`) (default 1)

datanorm: search on absolute normalisation of this dataset (default: 1.0)

Repeated `ndatasets` times, namelist with some of the following variables, then the corresponding data:

Card 3: (namelist: 'data')

type, data\_file, points, delta, xmin, lab, energy, angle,  
idir, iscale, abserr, ic, ia, k, q, jtot, par, channel, value, error,  
pel, exl, labe, lin, lex, ib

type (default 0)

= 0 angular distribution for fixed energy

= 1 excitation and angular cross section double distributions

= 2 excitation cross section for fixed angle

= 3 excitation total cross section. Also: `ic=0`: `ia=0` is total reaction cross section; `ia=1` is total fusion cross section;  $1 < ia < NFUS+1$  are fusion from potential KFUS (on Card 5) for inelastic state `ia-1`.

= 4 excitation phase shift for fixed partial wave

= 5 desired factor for bound state search (binding energy or potential scale according to ISC).

= 6 specific experimental constraint on a search parameter `par`, to be value with error `error` (`abserr=T` or `F`).

data\_file: name of data file with data, '=' for `search_file`, '<' for `stdin` (default '=')

points: number of data points (default: keep reading as many as possible),

delta: if non-zero, construct linear x-scale from `xmin` in steps of `delta`, (default 0)

lab: T or F for lab angles and cross sections (default F).

energy: lab energy for this `type=0` dataset (default: use `ELAB(1)` from Card 19)

pel, exl, labe, lin, lex: specify input channels for this data set, as in Card 18

idir (default 0)

= -1 cross-section data are given as astrophysical S-factors, but will be converted to absolute,

= 0 cross-section data are given in absolute units,

= 1 cross-section data are ratio to Rutherford

= 2 cross sections are given in absolute units but will be converted to ratio to rutherford.

iscale (default 2)

= -1 dimensionless (eg ratio to rutherford if `idir=1`),

= 0 absolute cross-section units are fermi-squared/sr.

= 1 absolute scale is barn/sr

= 2 absolute scale is mb/sr  
 = 3 absolute scale is micro-b/sr

abserr: T or F for absolute error (default F)

ic: partition number of cross section channel (index of Cards 6) (default 1)

ia: excitation pair number of cross section (index of Cards 7) (default 1)

k: tensor rank of cross section (0, 1, 2,...) (default 0).

q: index for tensor  $T_{kq}$  of cross section (0, 1, 2,...) (default 0).  $T_{00}$  = angular distribution  $\sigma(\theta)$ .

jtot: The J value (as on Card 2) for phase shift

par: The parity (-1 or +1) for phase shift, for type=4

par or number of search parameter, for type=6.

channel: Channel number of entrance channel in coupled channels set (default 1), for phase shift

value: Value of search parameter, for type=6

error: Error in value of search parameter, for type=6

ib: if  $0 < ib < ia$ , then ib is final state of gamma decay. (default 0)

If this is given for data type=0,1,2, then the ia is the initial state, and all angles are the *gamma* detection angles, and cross sections are integrated over all ejectile particle angles. Need to set dgam=1, pp=3, kqmax  $\geq 2 \times$  spin of state ia, thmin=0 and thmax=180 degrees.

#### Data input (free format):

if type=1, read: energy, angle, value, error

if type=5, read: kn, target, error

otherwise:

if delta  $\neq 0$ , read: value, error

if delta=0, read: x, value, error

where x is angle for type=0, and lab energy for type=2, 3 and 4.

#### SFresco Input

The inputs to SFresco are

Card 1: name of search\_file

Cards 2: repeatedly one of (in all upper or all lower case):

EX: exit

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 number var with step step.

SCAN var val1 val2 step: scan variable number var from value val1 to value val2 in steps of step.

SHOW: list all datasets with current predictions and  $\chi$  values.

PLOT plotfile: write file (default: search.plot) for reading by xmgr, xvgr, with data and theoretical curves.

LINE plotfile: write file (default: search.plot) for reading by xmgr, xvgr, with theoretical curves only.

READ file: read plot output file for further searches, if not:

READ snapfile: if the input string file contains the string 'snap', read to the end of previous snap output snapfile, for further searches.

ESCAN emin emax estep: scan lab. energy in incident channel, to give phase shifts in fort.71, fusion & reaction cross sections in fort.40, and S-factors in fort.35 and 75. This is to look for/at resonances, or at behaviour out of data's energy range, not for  $\chi^2$  fitting.

MIN: call minuit interactively, to read from stdin. Return to SFresco by minuit command end.

A example of this search\_file input is:

```
'6hep.in' '6hep.out' 7 1
&variable kind=1 name='V' kp=1 pline=2 col=1 /
&variable kind=1 name='r0' kp=1 pline=2 col=2 valmin=.7 valmax=2.0/
&variable kind=1 name='a' kp=1 pline=2 col=3 /
&variable kind=1 name='W' kp=1 pline=2 col=4 /
&variable kind=1 name='rw' kp=1 pline=2 col=5 valmin=.7 valmax=2.0/
&variable kind=1 name='aw' kp=1 pline=2 col=6 /
&variable kind=5 name='exptnorm' /
&data type=0 iscale=2 idir=0 lab=F abserr=T/
13.99      565.7      28.3
17.59      478.19     23.91
21.22      425.41     21.28
24.92      338.44     16.93
28.68      284.71     14.24
36.48      168.59      8.43
40.56      137.9       6.86
44.8       104.75      5.24
53.        30.0        9.14
53.94      38.45       2.71
59.        25.62       2.55
&
```

A example of the full SFresco input, suitable for batch running, is:

```
search4.in
min
fix 4
migrad
end
q
show
plot
```

where search4.in is the above search\_file input file name.

## Appendix VII : Stabilization method for coupled channels solutions

Antonio Moro has contributed a a stabilization algorithmn to solve or, at least, palliate, the common problem of loss of linear dependence of the coupled channels solutions. Following the suggestion of some Japanese researchers, he implemented a method of re-orthogonalization similar to that described in the papers of Baylis *et al*, but using a QR orthogonalization procedure instead of the Gram-Schmidt method used by them.

Thanks to this implementation, we are now able to solve efficiently problems which were otherwise not feasible, for example, CDCC calculations with high-lying breakup states, including closed-channels. His group to extend this to the case of transfer reactions, but only with limited success, so in practice it works only for pure coupled channels equations.

A test case `dNi-cdcc-QR.in` is included in the `test/` folder, corresponding to a  $d+^{58}\text{Ni}$  reaction at 20 MeV, including closed channels. In this case, the standard Numerov method fails for  $JT>3$ , whereas with the stabilization procedure the calculation runs smoothly for all required partial waves.

To activate this option we added a variable `hort` to the FRESKO namelist, which corresponds to the radial interval step at which stabilization is performed. Typically, try `hort = 5 fm`. This orthogonalizing continues out to the largest classical turning radius for any open channel, but can continued further by setting the radius variable `rmort` also in the FRESKO namelist.

WE. Baylis and S.J. Peel, Computer Physics Communications **25** (1982), 7-19,