

# Fresco

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## 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

A120 HEADNG

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

#### Card 1

10F8.4 HCM, RMATCH, RINTP, HNL, RNL, CENTRE, HNN, RNN, RMIN, RSP

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.

For two-nucleon transfers, the nucleon-nucleon distance is discretised from RMIN to RNN in a multiple of 6 Gaussian quadrature points to give step size approx. HNN.

When folding single-particle states (bound states or continuum bins) with KIND=3 or 4 couplings, the state radii are limited to RSP.

#### 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, A2, 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  $\max(0, JTMIN) < J < JTMAX$ , 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  $J < \text{abs}(JTMIN)$  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', include only negative parity coupled channels sets.

If CSET = 'N', include only natural parity coupled channels sets,

If CSET = 'U', include only unnatural parity coupled channels sets.

Here, 'natural parity' is defined as  $\text{parity} = (-1)^{\text{nint}(JTOTAL+1)}$ .

RELA ne ' ', use relativistic kinematics for the incident projectile:

If RELA contains 'a', use Ingemarsson eq(16) for kinematics

If RELA contains 'b', use Ingemarsson eq(17) for kinematics

If RELA contains 'h', use kinematics of G.Hale (LANL), EDA code

If RELA contains 'f', use Ingemarsson eq(19) to scale potentials

If RELA contains 'g', use Ingemarsson eq(21) to scale potentials

If RELA contains 'r', get reduced mass from ratios of total energies

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  $J \geq JBORD(i)$ , 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,F7.4,I1,3F8.4 KQMAX,PP,THMIN,THMAX,THINC,KOORDS,CUTL,CUTR,CUTC

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

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  $\max(\text{CUTL} \cdot \ell \cdot \text{HCM}, \text{CUTR})$ .

If CUTR < 0, put cutoff at point-Coulomb turning point  $-|\text{CUTR}|$ .

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, 2f8.6, i4, i2, l1, F8.4
ERANGE, DK, INH, plane, smallchan, smallcoup, NUMNODE, NTHREAD, CCREAL, ELPMAX
```

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  $(2J+1)/(2J_{TMAX}+1)$ ) 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  $\text{abs}(\text{ITER})$  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  $\text{abs}(\text{IPS})$ , 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,

= 2 for Pade acceleration by finding the N/D polynomials.

ISO

= 0 or blank, for no isocentrifugal approximations,

= A or J, for replacing all barriers by  $L = J_{total}$  barrier

= B or L, for replacing all barriers by  $L = L_{in}$  barrier.

Of course, the *simplest and fastest* way to use the isocentrifugal approximation is to put all spins and parities to  $0^+$ , and all transition multipoles to  $k = 0$ . The ISO variable is not needed then.

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  $|\text{JTMIN}|-6$ .

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  $(30/\text{NNU})^2\%$ .

ERANGE = range of energies of the upper and lower boundaries of continuum bins: if ERANGE > 0, then RATIO of these energies; if ERANGE < 0, then DIFFERENCE of the energies in MeV.

DK = step size of  $k$  ( $\text{fm}^{-1}$ ) for integration over the ERANGE to construct the continuum bin.

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.

NUMNODE = number of parallel nodes for MPI operation

NTHREAD = number of threads/node for OPENMP operation, so number of CPUS is NUMNODE\*NTHREAD

CCREAL = T: assume all potentials and couplings real-valued

ELPMAX = energy ELAB below which the LPMAX in each partition are applied

#### Card 4.5

If IBLOCK<0, then read:

```
2i4,          I1,      L1,      I2,  i2,      f6.4,  3f8.4,1x,A1
NRBASES,NRBMIN,BUTTLE,PRALPHA,PCON,MEIGS,RMATR,BNDX(2),WEAK,BTYPE
```

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

If NRBASES < 0, then use **Lagrange mesh** with NLAG=-NRBASES basis functions.

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.

BNDX(i) is used to set the R-matrix Boundary Condition number depending on BTYPE. Use i=1,2 for positive,negative parity coupled channels sets (respectively).

Energy  $\hbar^2 k^2 / 2m$ , where  $k = f'/f$ , the logarithmic derivative for all radial basis states at  $r=\text{RMATR}$ , with  $k$  having the same sign as EBETA(i).

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, MELFIL, C

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  $\geq 1$  : 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

$\geq 1$  : Print all potentials as they are calculated from Cards 10

$\geq 3$  : Print all potentials as they are calculated from Cards 9

CDETR

$\geq 1$  : Print information on the solving of the coupled equations. (decrement).

SMATS

$\geq 1$  : Print absorption & 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. Decrement.

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

- $\geq 1$  : 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  $VEFF \neq 0$ .
- $\geq 2$  : Print out L-distributions of the fusion cross section.

## MELFIL

- $\neq 0$  : Write real files 53 and 54 in the ‘mel’ and ‘spec’ format for use e.g. by R-matrix program `sturmx`.
- $= \pm 2$  : Write complex files 53 and 54 in the ‘mel’ and ‘spec’ format.
- $< 0$  : Write file 53 ‘mel’ in text format format.

CDCC = 1: Print out the  $f(m'M' : mM; \theta)$  for each angle  $\theta$  on file 57 for partition PEL, after the following information for *uncoupled* bin states:

```
card Y: (i2) 1      (indicating CDCC=1 format below)
card Z: (A120)  HEADNG from Fresco input card 0.
card A: (F10.4,3F8.4)  ENLAB,Bproj,H2SM,e^2,Btarg,inp, (Qval if inp=1)
                    lab energy,projectile binding energy, hbar^2/2.m, e^2,
                    target binding energy,inp, Qval if inp=1

card B: (7f8.4)      massp,masst,massc,massv,massr
                    masses: projectile,target,core,valence,residual

card C: (7f8.4)      Zp,Zt,Zc,Zv,Zr      charges
card D: (7A8)      namep,namet,namec,namev,namer names
card E: (7f8.1)      Jp,Jt,Jc,Jv,Jr      g.s. spins
card F: (7i8)      Pp,Pt,Pc,Pv,Pr      g.s. parities
    If inp=1, cards B-F (incl) have further #6 and #7 values
    for 'initial projectile' and 'initial target' too.

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)
        1,j,Emid,kmin,kmax,NK,KN,ISC
        1,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 (not including core spin)
        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 for all CDCC values 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.t

Summary of bin normalisation factors for different ISC values:

ISC

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

CDCC = 2: Print out the  $f(m'M' : mM; \theta)$  for each angle  $\theta$  on file 57 for partition PEL, after the following information for *coupled bin states*:

```

card Y: (i2)  2      (indicating CDCC=2 format below)
card Z: (A120)  HEADNG from Fresco input card 0.
card A: (F10.4,3F8.4)  ENLAB,Bproj,H2SM,e^2,Btarg,inp, Qval if inp=1
                        lab energy,projectile binding energy, hbar^2/2.m, e^2,
                        target binding energy,inp, Qval
card B: (7f8.4)      massp,masst,massc,massv,massr
                        masses: projectile,target,core,valence,residual
card C: (7f8.4)      Zp,Zt,Zc,Zv,Zr      charges
card D: (7A8)      namep,namet,namec,namev,namer names
card E: (7f8.1)      Jp,Jt,Jc,Jv,Jr      g.s. spins
card F: (7i8)      Pp,Pt,Pc,Pv,Pr      g.s. parities
    If inp=1, cards B-F (incl) have further #6 and #7 values
        for 'initial projectile' and 'initial target' too.

card G: (5I4)      NBINS,NKMAX,NEXB,NNJMAX,NCHMAX
                        no. CDCC bins, max NK,
                        no. excited states, max(2*Jex+1), max nch
card H: (I4,2f8.4)  NANGL,THMIN,THINC      (cm angular range from Card 3)
card I: (I4)      NCE      (number of excited states. NCE=0 for only gs).
for each of the ICE=1...NCE core excited states (card skipped if NCE=0)
cards J: (I4,2f8.4)  IPARCE, JCE, ECE      (parity -1,+1; spin; energy of excited states)
                        (for the gs: parity=Pc, spin=Jc, energy=0.0)
for each of the NBINS bins:
    card K: (f4.1,2I4,f4.1,3f8.4,2i4)
        Jex,Pex,nch,Emid,kmin,kmax,NK,KN,ISC
        Jex: overall spin [ (1 s)j, JCE(ICE); Jex>
        Pex: overall parity = parity(ICE) * (-1)**1
        nch: number of partial wave channels coupled to Jex/Pex.
        IL: incident channel (1<= IL <= nch)
        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 partial wave c=1..nch
        card L: (i4,f4.1,i4)
            l,j,ICE: quantum numbers. Use s=Jv.
    for each IK=1,NK for k=kmin+(IK-1)*kinc where kinc = (kmax-kmin)/(NK-1)
        card M: (2f10.6) delta(IK),k: any nuclear phase shift used in bin integral (radians)
        card N: (10f10.6) S(:, :) the full scattering S matrix for nch channels
                        (always nch*nch, so closed channels included)

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 (including core spin)
        Pex: parity of this projectile state
        Eex: excitation energy of this state above g.s. (including core energy)
        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)

```

## 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-  Qvalue
----projectile-----              -----target-----

I8,          F8.4,  2I4
READSTATES, PRMAX, LPMAX1(IC), MIXPOT

```

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.

If  $PRMAX \neq 0$ , then use  $PRMAX$  for matching radius in this partition

If  $LPMAX1 \geq 0$ , then  $LPMAX = LPMAX1 - 1$  is the maximum partial wave in this partition. Applied for incident energies ELAB below ELPMAX.

MIXPOT governs the couplings that are generated (in this partition) between levels that have *different* KP potential indices. It does not affect any couplings when the KP index values are identical.

$\leq 0$ : no couplings (default)

= 1: couplings only to or from the first state in that partition

= 2: couplings only according to the KP value of the destination level

= 3: all couplings produced by either KP value.

### 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(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

9	SHAPE	Effective mass: reduction from unity
0		Coulomb potential (see Card 9 above)
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.
14	SHAPE	Projectile second-order coupled by matrix elements read in.
15	SHAPE	Target second-order coupled by matrix elements read in.
16	SHAPE	Target & projectile simultaneous second-order coupled by matrix elements read in.

17		Target & projectile all-order coupled by matrix elements read in.
20	NUM	Super-soft N-N potl. of de Tournell & Sprung (SSC(C))
21	NUM	User-supplied N-N potential via subroutine NNPOT.
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 & 15) 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  $\text{CONLS} = \hbar^2 / (m_\pi^2 c^2) = 2.000$ .

- 0 : Woods-Saxon =  $-\text{CONLS} * \text{P1} * \text{E} / [(1+\text{E})^2 * \text{P3} * \text{r}]$
- 1 : WS squared =  $-\text{CONLS} * \text{P1} * \text{E} * \text{E} / (1+\text{E})^3 / (2 * \text{r} * \text{P3})$
- 2 : Gaussian =  $-\text{CONLS} * \text{P1} * \exp(-\text{RH} * \text{RH}) * \text{RH} / (2 * \text{r} * \text{P3})$
- 3 : Yukawa =  $-\text{CONLS} * \text{P1} * \text{E} * (1 + \text{r}/\text{P3}) / (4 * \text{r}^3 * \text{P3})$
- 4 : Exponential =  $-\text{CONLS} * \text{P1} * \text{E} / (4 * \text{r} * \text{P3})$
- 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  $\text{E}=1$ , if reasonable):

- 0 : Woods-Saxon =  $\text{P1} * 8 * \text{E} * (\text{E}-1) / (1+\text{E})^3$
- 1 : WS squared =  $\text{P1} * 4 * \text{E} * \text{E} / (1+\text{E})^3$
- 2 : Gaussian =  $\text{P1} * 2 * \exp(-\text{RH} * \text{RH}) * \text{RH}$
- 3 : Yukawa =  $\text{P1} * \text{E} * (1/\text{P3}^2 + 2/\text{r}^2) / \text{r}$
- 4 : Exponential =  $\text{P1} * \text{E}$
- 5 : Reid soft core, 12 \* tensor part
- 6 : Vol Gaussian =  $12 * \text{P1} * \exp(-\text{RH} * \text{RH})$
- 7,8,9 : Read from cards, as above.

If  $\text{SHAPE} \geq 30$ , 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 =  $1 / (1 + 1/\text{E})$ ,  
           =1 : WS squared =  $1 / (1 + 1/\text{E})^2$   
           =2 : Gaussian =  $\exp(-\text{RH}^2)$ ,  
           where  $\text{X}=\text{L}$  (for  $\text{JL}='L'$ ),  $\text{X}=\text{J}$  ( $\text{JL}='J'$ ),  $\text{RH} = (\text{X}-\text{XLVARY})/\text{ALVARY}$ , and  $\text{E}=\exp(-\text{RH})$ .

If  $\text{SHAPE} \geq 10$  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  $\text{SHAPE} \geq 20$ .

If  $\text{SHAPE} \geq 20$  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  $\text{M} = \text{RMATCH}/\text{HCM}+1$  complex numbers in FORMAT(6E12.4) from the file as a random-access set of card images, with  $(\text{M}-1)/3+1$  card images for each form factor.

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

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

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



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  $40 \leq \text{SHAPE} \leq 43$ . 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  $P(k) = \text{DEF}(k)$ , the deformation lengths (in fm.). ( $P0 = \text{DEF}(0)$  for *inelastic* monopoles.)

For Coulomb deformations  $P(k) = \text{Mn}(Ek)$ , the intrinsic reduced matrix elements in units of  $e.f.m^k$  ( $P0$  gives  $\text{Mn}(0)$  for *inelastic* monopoles). These intrinsic matrix elements  $\text{Mn}(Ek)$  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:

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

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

$\text{Mn}(E2)$  is related to the intrinsic quadrupole moment in the rotational model by  $\text{Mn}(Ek) = Q_0 \sqrt{5/16\pi}$ .

For a uniformly charged sphere of radius  $R$ , to first order in  $\beta_k$  we have

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

The  $\text{Mn}(Ek)$  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.

For TYPEs 14–17, 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. Only nuclear couplings are yet implemented.

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. For TYPEs=14–17, the IB and IA can reference any combination of projectile and target states, but  $k > 0$  for projectile and  $k < 0$  for target states. STR refers to the RDEF(k) measure above; the factor  $(-1)^{[I-I'+|I-I'|]/2}$  must be included. The SHAPE and P0-P6 parameters on the TYPE=17 card 10 are not used.

For TYPE=17, couplings, to all orders in RDEF, are calculated between all pairs of projectile and target states using the matrix eigensolution method of Kermode and Rowley, Phys. Rev. **C48** (1993) 2326.

## 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,F8.4
KBPOT,KRPOT, BE,    ISC,IPC,  NFL,  NAM,AMPL,  NK,ER

```

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 coupling order (0 to 4 for one-particle states, and 6 to 9 for two-particle states) :

- = 0 for  $(LN,SN) JN$  couplings ← use for typical transfers
- = 1 for  $|L_n, (SN, J_{core}) S; J_{com}\rangle$  (IA & IB must be given) \*
- = 2 for eigenstate in deformed potential (fixed SN, K, Parity) \*
- = 3 for  $|(LN, SN) Jn, J_{core}; J_{com}\rangle$  (IA & IB must be given)
- = 4 for form of leg of the Dalitz-Thacker Triton
- = 5 (not used)
- = 6 for  $|L_{nn}, (\ell, S_{12}) j_{12}; J_{12}\rangle$  with isospin  $(.5, .5)T$
- = 7 for  $|(L_{nn}, \ell) L_t, (S_{12}, J_{core}) S_t; J_{com}\rangle$  &  $|( .5, .5) T, T_{core}; T_{com}\rangle$  \*
- = 8 (not used)
- = 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)
- $K_{core}$  = projection K of core nucleus (state IA)
- $K_{com}$  = projection K of composite nucleus (state IB)
- $T_{core}$  = isospin of core nucleus (state IA)
- $T_{com}$  = isospin of composite nucleus (state IB)

and \* signifies that transfers using these KINDs are not yet implemented.

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 (KINDs 6 & 9)

= combined cluster and core intrinsic spins (KIND 7)

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

JN = vector sum LN + SN,

but for KIND=1,  $JN = SN + J_{core}$  (i.e. S in LS coupling)

and for KIND=7,  $JN = L_{nn} + \ell$  (i.e. L in LS coupling)

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

KBOT = 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 KBOT. 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)

### BOUND STATES:

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

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

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

### 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  $\text{ISC} > 0$  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. KIND=3 and 4 forward and reverse couplings are both calculated explicitly, but not 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 `abs(RMATCH)` and `RASYM` in the `CRCWFN` calculations (the values on Card 1a).

In general,  $\text{ISC}=2$  is recommended (or  $\text{ISC}=4$  for resonances), since then the coupled-channels bins will be nearly real. With  $\text{ISC}=-2$  (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 information:

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 = 1,  $L_n, (SN, J_{core})S; J_{com}$  i.e. LS coupling.

Coupled form factors with sum over  $L_n$  and  $S$ .

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

IA giving  $J_{core}$ , spin of core nucleus.

IB giving  $J_{com}$ , spin of composite nucleus.

LMAX is maximum  $L_n$  in summation.

JN is maximum  $S$  in summation.

NN & L restrict the number of radial nodes of one component wave function in the coupled set :

NN gives the number of radial nodes of the last partial wave of angular momentum  $L_n = L$  input.

For KIND = 2, eigenstates in a deformed potential, for fixed parity and K projection :

Coupled form factors  $(l_n, SN)JN, K$ , with sum over  $L_n$  &  $J_n$ .

SN, LMAX, NN & L are as for KIND = 1 :

SN as read in, the intrinsic spin of the bound particle. LMAX is maximum  $L_n$  in summation. NN & L restrict the number of radial nodes of one component wave function in the coupled set.

IA is a core state with correct  $K_{core}$  projection quantum number.

IB is a composite state with correct  $K_{com}$  projection number.

so  $K = K_{com} - K_{core}$

JN is the maximum Jn in the summation.

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

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

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 Jn 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.





## 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 : general partial-wave couplings
- = 10 : (spare)
- = 11 : Projectile-valence non-orthogonality
- = 12 : Target-valence non-orthogonality (not implemented)

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 'INFILE' [default 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.  
 -4 : call subroutine FNLREAD to read in non-local form factor, and multiplying it by the Racah-algebra factor in Appendix V (except for the  $1/\sqrt{4\pi}$  factor) for given IB, IA final and initial excited states. The order of form factors in the file must agree with the order called by a double loop of channels, with the 'to' channel number varying more rapidly.  
 -5 : call subroutine FNLREAD to read in non-local form factor for given IB, IA final and initial excited states. The order of form factors in the file must agree with the order called by a double loop of channels, with the 'to' channel number varying more rapidly.

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

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

```
Card 16.2: 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 16.2, 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 = 0,4 : Calculates both electric and magnetic couplings (reads  $g$ -factors from P1&P2)

1,5 : for electric only

2 : for magnetic only (reads  $g$ -factors from P1&P2)

4,5 : include also Siegert remnant for electric transitions

IP3: *not implemented yet*

P1 = projectile *g*-factor

P2 = target *g*-factor

IP4 = 0 : direct capture only

1 : semi-direct capture only

2 : direct + semi-direct capture mechanisms.

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

IP5 =  $\Lambda_{\text{max}}$ , 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

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)  
 2 : Surface transfer operator, on surface if *final* bound state  $r' = P1$ . IP2 and IP3 ignored.  
 3 : Surface transfer operator, on surface if *initial* bound state  $r = P1$ . (Not yet implemented)  
 4 : Surface transfer operator calculated as PRIOR–POST. Need also to set RSMAX for *final* bound state to the desired surface radius. (Implemented, but not yet correctly).  
 5 : Surface transfer operator calculated as POST–PRIOR. Need also to set RSMAX for *initial* bound state to the desired surface radius. (Not yet implemented).

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 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.

KIND = 9 : General Partial-Wave Couplings (local or non-local external interactions from FILE ‘INFILE’ [default 4])

IP1 = 0 : local form factor  
 1 : non-local (two-dimensional) form factor

IP2 = 0 : read in real values  
 1 : read in imaginary values  
 2 : read in complex values

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

For IP1=0 (local), read from file ‘INFILE’ the following cards (until a blank card):

Card 16.6: (free format) NP , HNP, RFS

for NP = number of radial points  
HNP = step size  
RFS = radius of first point

For IP1=1 (nonlocal), read from file 'INFILE' the following cards (until a blank card):

Card 16.7: (free format)                      NLLI, RINTPI, NLOI, HNLI, NLCI  
for NLLI = number of radial points in R  
RINTPI = step size in R  
NLOI = number of radial points in  $D=R'-R$   
HNLI= step size in D  
NLCI=offset index for  $D=0$

Card 16.8

F8.1, I4,                      2I4, f6.1,                      2I4, F6.1                      L2  
JTOTAL, PARITY, IB, LVAL1, JVAL1, IA, LVAL2, JVAL2, REV

each with following potential data of Cards 16.6 or 16.7. These are the couplings from partial wave *to* (LVAL1,JVAL1) for excited state pair IB *from* partial wave (LVAL2,JVAL2) for excited state pair IA, in coupled channels set JTOTAL of parity PARITY (+1 or -1). The reverse coupling is also included if REV is true.

If IB or IA is zero, match any state. If JVALi < 0, then match any JVALi. If PARITY=0, match any parity. If JTOTAL<0, match any JTOTAL. If LVALi < 0, then match any LVALi. If LVAL1=LVAL2<0, then require partial wave coupling to be diagonal for equal  $LVAL=-LVALi-1$ .

For IP1=0 (local),

read (free format) NP values

For IP1=1 (nonlocal), read NLLI loops of:

read NLOI values (free format).

Go back to reading cards 16.6 or 16.7 (though subsequent values on those cards are ignored).

KIND = 11 : Projectile-valence non-orthogonality Construct non-orthogonality overlap, for use in R-matrix or Lagrange-mesh methods, for the case when a projectile *p* scattering on a target consisting of {core *c* + valence *v*} can be rearranged in another partition to be projectile' *v* scattering on a target' consisting of {core *c* + valence *p*}.

ICTO, ICFROM are the two partitions with *p* and *v* as projectiles (either order).

IP1 = ICORE is the partition in which the target is the bare core *c*.

Spectroscopic amplitudes need to have been defined for  $\langle c|c+v=t \rangle$  and  $\langle c|c+p=t' \rangle$ . NO amplitudes like Cards 17 are to be read in after this coupling.

The reverse case (KIND=12), where the projectile is composite rather than the target, is not yet implemented.

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 FRESKO 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.

A utility routine fr2nl.f is provided which will convert card-image line input to the new namelist input. Please check that your input numbers have sufficient range and accuracy in the formats chosen for the namelists, and that 'unitmass' is correct for your masses (see discussion below).

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, hnn, rnn, rmin, rasym, accrcy, switch,  
ajswtch,  
jtmin, jtmax, absend, dry, rela, nearfa,  
kqmax, pp, thmin, thmax, thinc, koords, cutl, cutr, cutc, elpmax,  
nrbases, nrbmin, buttle, pralpha, pcon, meigs, rmatr, ebeta,  
ips, it0, iter, iblock, pade, iso, nnu, maxl, minl, mtmin, epc, erange, dk,  
inh, plane, smallchan, smallcoup,  
chans, listcc, treneg, cdetr, smats, xstabl, nlpl, waves, lampl, veff, kfus,  
wdisk, bpm, melfil,  
pel, exl, lab, lin, lex, elab, nlab  
along with new variables fatal, nosol, nangle, 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).

nangle = number of additional angle in ANGLE(:) for cross sections. (setting of ANGLE(:) is not yet implemented)

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	aso
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 defn(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 to override erange). That is, 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 ← - 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 ← kfrag, and if(kcore>0) p2 ← 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 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, rasy, 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  $h=H_{CM}$  and  $K$  is the elastic wave number. (default hktarg=0.2).  
If  $H_{CM}=0$  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, B and p/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(rojectile) 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 ncou=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)	Common suffix	Routines	Use
1	V			SFRESKO	FRESKO input when searching
2	V			SFRESKO	Search specification file
3	V			FREADF, FR	Temporary namelist file
4	F	80		INTER POTENT	default for external KIND=1,9 couplings external potentials
5	F	80	in		standard input
6	V	133	out		standard output
7	F	80	smats	DISPX	elastic S-matrix elements
8 #	F	sector	(tmp)	FR,INTER	s/p wfs, channel wfs
9 #	F	NLL*NLO*16	(tmp)	Q/KERNEL	complex transfer multipoles
10 @	V		(tmp)	FR,CRISS	S-matrix elements (cfs)
11 #	F	NLL*NLO*8	(tmp)	Q/KERNEL	real transfer multipole
12 #	V	NLL*NLO*16	(tmp)	KERNEL/SOURCE	transfer kernels
13	F	80	xst	FR	total cross sections for each Elab
14 #	V			INTER/CPAIR	interaction potentials
15	V		(tmp)	FR	local equivalent potent
16	F	80	xsec	CRISS	tables of cross sections
17	F	80	swf	FR	output scattering waves
18 #	V		(tmp)	FR	wfns of 'best' iterate
19	F	N		FR	Local couplings
20–33				Available for users	(eg bound states, amplitudes, potentials)
34	F	80		POTENT	output potentials
35	F	80	sf	FR	Astrophysical S-factors for Ecm
36				CRISS	output scattering AMPL amplitudes
37				CRISS	output scattering FAM amplitudes
38	F	80		DISPX	cross sections for each J/pi
39	F	80	efus	FR	2 cross sections for each Elab
40	F	80	fus	FR	all cross sections for each Elab
41	F	80		SOURCE	source terms at each iteration
42	F	80		SOURCE	bin wavefunctions for each E
43	F	80		INFORM	bin phase shifts as k functions
44	F	80	phe	INFORM	bin phase shifts as E functions
45	F	80		ERWIN	scat phase shift as E functions
46	F	80		INFORM	bs wave functions & Whit ratios
47	F	80	mek		reduced matrix elements
48 #	V	133		FR	concurrency log file
49 #	V			FR,CRISS	S-matrix elements concurrent→10

File no.	Format (Fix/Var)	LRECL (bytes)	Access (Seq/Ran)	Routines	Use
50 #	V	133			tmp standard output concurrent→6
51,52 #	V	133			unwanted standard output for node N>0
53	V		mel	WRITEMEL	mel file for sturmx(x)
54	V		spec	WRITESPEC	spec file for sturmx(x)
55	F			INFORM	Single-particle wave functions
56	F		fusl	FR	Jtotal fusion & reaction cross
57	F		cdcc	FR	Output of CDCC amplitudes
58	F		wfs	INFORM	Bound state wave functions
59	F		vert	INFORM	Bound state vertex functions
60-62	F		imp	RMATRIX	Trace of R-matrix calculations
63	F			WRITEMEL	Asymptotic coupling coefficients
64	F			RMATRIX	Coupled eigenstates
65 #	F	NLO*2*8	(tmp)	QNN	two-particle multipoles
66	V	NLL*NLO*16		INTER	KIND=1 nonlocal formfactor
70	F			RMATRIX	Basis state wfs
71	F	132	phs	FR	20 pw phase shifts as Elab functions
79+CP	V	{N,NLN*NLO}*16	(tmp)	INTER/KERNEL	(non)local partial-wave couplings
87	V		pnl	KERNEL	Non-local couplings
88	F			RMATRIX	Bound state wfs
89	F			MULTIP	Folded coupling potentials
90	V		veff	FR	average local equivalent potential
91	V		vpol	FR	average LEP for rereadingl
92	F			FR	Partial fusion cross sections
99	F	80		CRISS	input J/L rescaling factors
105	V			FCN	$\chi^2$ progress during fitting
200	F	80	xsel	CRISS	Elastic cross section if not fort.201
201-210	F	80	xs[1-9]	CRISS	Cross sections (cf 14) for states 1-10
301	V			CDCIN	New Fresco input
302	V			CDCIN	New Fresco input (temp)
303	V			SFRESKO	Input search file
304	V			SFRESKO	Output plot file
305	V			CDCIN	New Fresco input from cdcin, col format
306	V			SFRESKO/FRXX0	Input Fresco file
307	V			SFRESKO/FRXX0	Initial Output Fresco file
308	V			SFRESKO/FRXX0	Main Output Fresco file
470+i	V			erwinmpi	Log files from MPI process <i>i</i>

where for MACH=8 we have

# = distributed file: distinct file name on each node

@ = shared concurrent file: single file, with writes from each node

The use of files 19 and 35 have recently changed.

## 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

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

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 16.2.

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 an program which search 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, kp, pline, col, potential,
dataset, datanorm, dataEshift, reffile, nafrac, afrac,
energy, damp, jtot, par, channel, width, rwa, leff
```

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)  
damp: energy (cm MeV in entrance channel) of imaginary width of this R-matrix term (default 0).  
The actual imaginary part is damp/2  
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 FRESKO)  
term: term number (default 1)  
rwa: the width is reduced width amplitude  $\gamma$ , else  $\Gamma = 2\gamma^2 P$ . (default T)  
B: the boundary condition B. (Default: from BNDX).  
width: width for this channel (MeV<sup>1/2</sup> if rwa or energy subthreshold, else MeV(cm)) (default 0)

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

dataset (1:2): index (or, first and last, inclusive) of which dataset (1 to ndatasets) (default 1), or  
reffile: filename of dataset. If has a '\*', renorm all sets with names matching up to that character,  
datanorm: search on absolute normalisation factor of this dataset and its error (default: 1.0)

**kind=6: Variable dataset energy shift:**

dataset (1:2): index (or, first and last, inclusive) of which dataset (1 to ndatasets) (default 1), or  
reffile: filename of dataset. If has a '\*', shift all sets with names matching up to that character,  
dataEshift: search on absolute energy incremental shift of this dataset (default: 0.0)

**kind=7: Variable damping width of R-matrix term:**

term: term (default 1). For the real energy there should be a kind=3 variable with the same term.  
damp: Imaginary width (cm MeV in entrance channel) of this R-matrix term (default 0).  
When energy is set, use the (real) leff to rescale the damping width according to energy above threshold energy by the penetrability ratio  $P_{\text{eff}}(E - \text{energy})/P_{\text{eff}}(e_{\text{pole}} - \text{energy})$ , with elastic Coulomb. If not set, use constant damping widths as 2\*imaginary parts of the pole energies.  
The damp variable in kind=3 is fixed, but those in kind=7 can be varied in searches.

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,iscala,abserr,ic,ia,k,q,jtot,par,channel,value,error,leg,
pel,exl,labe,lin,lex,term
```

type (default 0)

- = -3 Legendre coefficient for input energy and fixed order leg
- = -2 Legendre coefficient (integer order leg) for input energy: double distribution
- = -1 Legendre coefficient for varying integer order leg, for fixed energy
- = 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  $F$ ).  
 = 7 specific constraint on energy of R-matrix pole term in the Brune basis to be value with error  $error$  ( $abserr=T$  or  $F$ ).  
 = 8 specific constraint on total formal width of R-matrix pole term in the Brune basis 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 for lab angles and cross sections (default F for cm frame).  
 $Aflip$ : T to change cm calculated angles to  $180 - \theta$  (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  $type=6$

**Data input (free format):**

```

if type=1 or -2, read: energy, angle, value, error
if type=5, read: kn, target, error
otherwise:
if delta≠0, read: value, error
if delta=0, read: x, value, error
  where x is angle for type=0, is leg for type=-1 or -2, and lab energy for type=-3, 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
V: query status of unfixed search variables
CHA: query status of changed search variables
CHI: list  $\chi^2$  status by dataset
SET var val: set variable number var to value val.
FIX var: fix variable number var (set step=0).
FXWID : fix all R-matrix widths variables.
FXRPE : fix all R-matrix pole energy variables.
FXPBG : fix all pole energies variables with 'BG' in their name.
FXBG : fix all variables with 'BG' in their name.
FXNOR : fix all dataset norm variables (kind=5)
FXSHF : fix all dataset energy shift variables (kind=6)
FREE : free all R-matrix energies and widths variables.
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.
DONE search_file: write single new search file (default: done.fresco) for reread-
ing by SFRESCO as a combination of FRESCO input_file and current parameter values.
Data specifications are however not included.
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.
ELIM emin emax: restrict data scans to this energy range for plots and  $\chi^2$  sums
POLES emin emax: vary only R-matrix poles in this energy range (others are fixed)

```



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.