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

$$S(R_f) = \int_0^{R_{match}} K_{fi}(R_f, R_i) u(R_i) dR_i \tag{1}$$

where RMATCH and HCM, the step size, are given in the &Fresco namelist. 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 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 card-image format

Please see document fresco-inputs.pdf.

3   Input NAMELIST format

The namelist input has two fixed-format lines to start with, and these followed by the namelists in Fortran style free-format. Variable names may be upper or lower case without distinction, but in this manual they are all capitalized. All namelists are terminated by a **/**. Some systems trailing comments begun by a **!**.

3.1   Initial Lines

Header line

One line of text to describe the nature of this run, for user's information only. (120 characters max)

NAMELIST

Fixed string to indicate input format using namelists

3.2   The &FRESCO namelist

Complete list of variables

Radial coordinates: hcm, rmatch, rintp, hnl, rnl, centre, hnn, rnn, rmin, rsp, cutl, cutr, cutc, rasym, accrcy, switch, sinjmax, ajswtch,

Partial waves: jtmin, jtmax, absend, jump, jbord, pset, jset, iso, llmax,

Angular distributions: kqmax, thmin, thmax, thinc, pp, koords, nearfa,

Defining coupled equations: inh, nnu, maxl, minl, mtmin, epc, erange, dk, plane, rela, ccbins, complexbins, sumform, pluto, unitmass, finec,

Incident channel: pel, exl, lab, lin, lex, elab, nlab,

Solving equations: ips, it0, iter, fatal, iblock, pade, nosol, dry, smallchan, smallcoup, hort, rmort, psiren, initwf, maxcoup, expand,

R-matrix setup: nrbases, nrbmin, pralpha, pcon, rmatr, btype, ebeta, buttle, weak, nparameters,

Trace variables: chans, listcc, treneg, cdetr, smats,

Output details: xstabl, nlpl, waves, lampl, veff, kfus, nfus, wdisk, bpm, melfil, cdcc, tmp

3.2.1   Radial coordinates

HCM, RMATCH, RINTP, HNL, RNL, CENTRE, HNN, RNN, RMIN, RSP, CUTL, CUTR, CUTC

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

If RMATCH < 0, then use values of RASYM, ACCRCY, SWITCH, AJSWITCH 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 discretized from RMIN to RNN in a multiple of 6 Gaussian quadrature points to give step size close to HNN.

RSP is the upper limit of state radius when folding single-particle states (bound states or continuum bins) with KIND=3 or 4 couplings.

CUTL: set the number of radial points per ℓ of the lower radial cutoff when integrating the radial equations. Default = −1.6
When CUTL>0, use $\ell = J$ (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 analyzing powers.

CUTR = lower radial cutoff (fm). Combining with CUTL is to use $R_{\min} = $ max(CUTL*ℓ*HCM,CUTR). If CUTR < 0, put cutoff at point-Coulomb turning point $-|$CUTR$|$.

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

RASYM, ACCRCY, SWITCH, SINJMAX, 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.

ACCRCY 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. If SINJMAX> 0, then change switchover condition to $J >$ SINJMAX.

AJSWITCH 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 $J \geq$AJSWITCH. Default is 0.0

3.2.2 Partial waves

JTMIN, JTMAX, ABSEND, JLEAST 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 JLEAST> 0, then only stop if $J >$ JLEAST.
If JTMIN < 0, then for $J <$ 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.

JUMP(1:), JBORD(1:) 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(0)=1 & JBORD(0)=JTMIN, and, if there are NJ non-zero values, also JBORD(NJ+1)=JTMAX. This gives no J jumping if JUMP and JBORD are not set in the namelist.) The omitted J values are provided by interpolation on the scattering amplitudes $A(m'M' : mM;L)$ prior to calculating cross sections.

PSET, JSET

If PSET = –1 or +1, restrict parity of CRC sets to that value (0 = no restriction)

JSET = number of CRC sets to calculate before stopping (0 = all sets)

ISO = 'A' or 'J', for replacing all barriers $L(L+1)$ by that for $L = J$ barrier
= 'B' or 'L', for replacing all barriers by $L = L_{in}$ barrier.
= 0 or blank, for no isocentrifugal approximations,

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.

LLMAX Maximum partial wave L in any CRC set.

3.2.3 Angular distributions

KQMAX, THMIN, THMAX, THINC Give cross sections (and tensor analyzing powers up to rank K = KQMAX) for centre-of-mass scattering angle from THMIN to abs(THMAX) in steps of THINC.
Elastic channels normally output the ratio to Rutherford, unless THMAX < 0.

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

KOORDS determines the coordinate systems used for the analyzing powers:
= 0 : Madison coordinates (default)
= 1 : Madison + Transverse
= 2 : Madison + Transverse + Recoil
= 3 : Madison + Transverse + Recoil + Hooton-Johnson

NEARFA For mod(NEARFA,10) values:
= 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.
If abs(NEARFA)$>$10, also split the Coulomb amplitude according to Cha, CPC 176 (2007) 318.

COMPLEXBINS, CCBINS

If COMPLEXBINS=T, allow for complex-valued bins (e.g. from optical potentials)
If CCBINS=T, allow for coupled-channels bins, which are necessarily complex-valued.

3.2.4 Defining coupled equations

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.

NNU, MAXL, MINL, MTMIN, EPC control the accuracy of non-local transfer form factors:

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

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

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

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

ERANGE, DK set default parameters for continuum bins:

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 (fm^{-1}) for integration over the ERANGE to construct the continuum bin.

PLANE
   = 1, 3: zero Coulomb potential for elastic channel
   = 2, 3: zero Coulomb potentials for all nonelastic channels.

RELA, RELREF $\neq$": 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 'c' or '3d', options for knockout reactions
   If RELA contains 'na' to use potential factor γ for inhomogenous terms.

PLUTO(:) = list of potential numbers KP to be prepared for the Lagrange-mesh method for single-particle eigenstates.

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

FINEC : 1/(fine-structure constant): used to determine electrostatic e^2. Default = 137.03599.

3.2.5 Incident channel

PEL, EXL, LAB, LIN, LEX Incoming plane waves are present in partition PEL with excitation pair EXL. The energies ELAB(:) 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 these variables can be normally omitted.

ELAB(:5), NLAB(:4) : Solve at different laboratory energies E until ELAB(i) = 0 is found.
If NLAB(i) > 1, then the range of E from ELAB(i) to ELAB(i+1) is covered in NLAB(i) linear intervals.
For just one energy E, just specify 'ELAB = E'.

3.2.6 Solving equations

IPS, IT0, ITER, FATAL, IBLOCK, PADE Solve the coupled channels equations by at least IT0 iterations, and up to ITER iterations. Stop sooner if the absolute differences between successive S-matrix elements (scaled by (2J+1)/(2.JTMAX+1)) are less than IPS percent. (Excited state pairs with IGNORE set in the &STATE namelist 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 FATAL=False allows continuation even after convergence has failed after abs(ITER) iterations.

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

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

PADE = 0 for no Pade acceleration,
= 1 for Pade acceleration by the epsilon algorithm,
= 2 for Pade acceleration by finding the N/D polynomials.

HORT, RMORT
HORT = radial interval step at which QR stabilization is performed
RMORT = radius outside classical turning point to which to extend orthogonalizing.
See section 9 for more details.

NOSOL : if not to solve the CRC equations, only construct couplings

DRY 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.

SMALLCHAN, SMALLCOUP
SMALLCHAN = fraction of unitarity to define a 'small channel'. A channel that is 'small' for NSMALL=5 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.

PSIREN : do simple renormalisation of channel wfs after Pade acceleration

INITWF : read in external scattering wave functions before iterating couplings. > 0: read in formatted data from file number INITWF.

< 0: read in unformatted data from file number INITWF.
The file format is that which is produced when WAVES> 0. All channels not read in are set to zero.

MAXCOUP(:), EXPAND(:) : fudge limits and factors (respectively) to adjust sizes of generated work arrays.

3.2.7 R-matrix setup

NRBASES

When NRBASES≠0, R-matrix solutions are selected then all channels are 'blocked' together and solved in a full CRC procedure. All non-local potentials are included to all all orders (not iteratively).

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* basis with NLAG=–NRBASES basis functions.

NRBMIN, BUTTLE, PRALPHA, PCON, RMATR, EBETA, WEAK, BES

NRBMIN = minimum number of radial basis states (default NRBASES).

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 for single-particle bound states).

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

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

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

NPARAMETERS Read in this number of R-matrix parameter namelists after the &FRESCO namelist.

3.2.8 Trace variables

A value of 0 gives no trace, increasing values give progressively more printed output.
Decremented variables are decreased by 1 on each use.

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

LISTCC = 1 : Print coupling coefficients between these channels. Decremented.
= 1,2,... Print progressively more detail of couplings.

TRENEG ≥ 1 : Print all multipole potentials
≥ 3 : Print all monopole potentials as well

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

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

≥ 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.

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

≥ 4 : Always print all the S-matrix elements.

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

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

3.2.9 Output details

XSTABL, NLPL, WAVES, LAMPL, VEFF, KFUS, NFUS, WDISK, BPM, MELFIL, CDCC, TCFILE

XSTABL $\neq 0$: If XSTABL is non-zero, in file 16 punch output cross sections for all excitation levels in all partitions. A header line in FORMAT(5I6) gives partition IC, level pair IA, number of tensor ranks of analyzing 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 in the &Fresco namelist are adequate. Decremented.

WAVES ± 1 or ± 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 θ.
<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 be averaging the 'trivially equivalent potential' over all the J, π 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 If KFUS > 0 : Calculate 'core fusion' using the imaginary and scalar parts of potential number KFUS (i.e.&pot namelists 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 :

```
line 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
line 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 lines 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.

```
line C: (6E12.4)   (psi(I),I=1,NR)   wave function
line C is repeated until NR complex values given
NB: the first point psi(1) = 0 always, as at r=0
```

Lines B & C are repeated for each channel, until IT < 0.
When WDISK < 0, successive records contain the two real values of psi(I), starting IN THIS CASE, from I=2 (i.e. $r = h$).

BPM ≥ 1 : Calculate fusion cross sections in the Barrier Penetration Model using first the bare potential, and then the bare potential + the 'weighted equivalent potential' calculated when VEFF $\neq 0$.
≥ 2 : Print out *L*-distributions of the fusion cross section.

MELFIL $\neq 0$: Write real files 53 and 54 in the 'mel' and 'spec' format for use e.g. by R-matrix program `sturmxx`.
$= \pm 2$: 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 θ on file 57 for partition `PEL`, after the following information for *uncoupled* bin states:

```
line Y:(i2)  1    (indicating CDCC=1 format below)
line Z: (A120)   HEADNG from Fresco input.
line 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

line B: (7f8.4)        massp,masst,massc,massv,massr
```

```
                                       masses: projectile,target,core,valence,residual
line C: (7f8.4)        Zp,Zt,Zc,Zv,Zr                charges
line D: (7A8)          namep,namet,namec,namev,namer names
line E: (7f8.1)        Jp,Jt,Jc,Jv,Jr               g.s. spins
line 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.


line G: (4I4)          NBINS,NKMAX,NEXB,NNJMAX no. CDCC bins, max NK,
                                            no. excited states, max(2*Jex+1)
line H: (I4,2f8.4)     NANGL,THMIN,THINC      (cm angular range from \&FRESCO)
for each of the NBINS bins:
 line I:(i2,2f4.1,3f8.4,2i4)
        l,j,Emid,kmin,kmax,NK,KN,ISC
            l,j: quantum numbers  (s==Jv)
            Emid:  centre of bin with respect to continuum threshold
            kmin,kmax,NK: Min,max and number of k values in bin integral
            KN:  original KN index for bin state
            ISC:  normalisation used for bin
     for each IK=1,NK
        line 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::
    line 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:
    line 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

= 2: $\exp(-i\delta(k))$
= 4: $\sin(\delta(k))\exp(-i\delta(k))$
= 12: $k\exp(-i\delta(k))$
= 14: $k\sin(\delta(k))\exp(-i\delta(k))$

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

```
line Y:(i2)  2    (indicating CDCC=2 format below)
line Z: (A120)   HEADNG from Fresco input.
line 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
line B: (7f8.4)        massp,masst,massc,massv,massr
                                       masses: projectile,target,core,valence,residual
line C: (7f8.4)        Zp,Zt,Zc,Zv,Zr                charges
```

```
line D: (7A8)            namep,namet,namec,namev,namer names
line E: (7f8.1)          Jp,Jt,Jc,Jv,Jr                g.s. spins
line 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.

line G: (5I4)            NBINS,NKMAX,NEXB,NNJMAX,NCHMAX
                                           no. CDCC bins, max NK,
                                           no. excited states, max(2*Jex+1), max nch
line H: (I4,2f8.4)       NANGL,THMIN,THINC     (cm angular range from \&FRESCO)
line 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)
lines 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  [ (l s)j, JCE(ICE); Jex>
           Pex: overall parity = parity(ICE) * (-1)**l
           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
       line 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)
       line M: (2f10.6) delta(IK),k: any nuclear phase shift used in bin integral (radians)
       line 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::
    line 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:
    line L: (6E12.4): ((FAM(MEX,MP,IANG,IA),MEX=1,2*Jex(IA)+1),MP=1,2*Jp+1)
```

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

3.3   &PARTITION and &STATES namelists

The &PARTITION namelists are repeated until an empty &PARTITION namelist is read in. After each non-empty (NEX > 0) &PARTITION, NEX instances of the &STATES namelist are required.

3.3.1   &PARTITION namelist

NAMEP, MASSP, ZP, and NAMET, MASST, ZT
   NAMEP = name of projectile-like nuclide (string 8 characters max),

MASSP = mass of projectile (in units of UNITMASS),

ZP = charge of nuclide,

NAMET, MASST, ZT = equivalent properties of target-like nuclide.

NEX, QVAL, PWF

abs(NEX) = number of excited-state pairs in this partition.

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

QVAL = Q-value (in MeV) of this partition for Ep+Et=0.0. Only differences in Q-values between partitions are significant.

PWF = use asymptotic piecewise methods in this partition (default is True).

READSTATES

read in specification of the NEX states from file number READSTATES.

PRMAX = maximum radius in this partition. Useful for R-matrix calculations, but redefines what 'local' interactions mean.

3.3.2 &STATES namelists

Repeated IA = 1,..,NEX times before the next &PARTITION:

Jp, COPYp, BANDp , Ep, KKp, Tp,   Jt, COPYt, BANDt , Et, KKt, Tt

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

J = spin of the state (Jp and Jt, and similarly below).

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. Odd multipoles couple BAND values of opposite sign.

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 (in &cfp namelists) 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))

KP, FEXCH,IGNORE, INFAM,OUTFAM

KP = index of optical potential for this pair of excited states. If zero, use as default KP = IC, the number of this partition.

If FEXCH = 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 above).

If INFAM $\neq$ 0, read in complex amplitudes later to add to calculated scattering amplitudes
< 0, read in only one amplitude (non spin-flip) for each scattering angle, with others zero.

If OUTFAM $\neq$ 0, write out complex amplitudes later to add to calculated scattering amplitudes.
< 0: write out only one amplitude for each angle, namely the average of diagonal amplitudes.

The output files are suitable to be reread later as input file

3.4 &POT potential namelists

Each potential is started by a &pot namelist with TYPE=0, defining the radii to be used and the diagonal Coulomb potential, followed by any number of further &pot namelists with TYPE>0, which cumulatively construct the components of the nuclear potential. The KP value in each namelist identifies the potential of which this is to be a component. The &pot namelists are repeated until KP< 0 indicates the last one to be considered, or an empty namelist is read in.

3.4.1 First kind of &pot namelist

KP, TYPE, p1, p2, p3, p4 with TYPE=0, or

KP, TYPE, AT, AP, RC, AC with TYPE=0 :
> All the radii are multiplied by CC.
> CC is updated by a TYPE=0 &pot namelist to CC = $AT^{1/3}$ + $AP^{1/3}$ where AT≡p1 and AP≡p2,
> CC is updated by TYPE>0 namelists, if P0 > 0, to CC = $P0^{1/3}$.
>
> RC≡p3 = surface radius (when multiplied by CC) of charge distribution
> AC≡p4 = diffuseness of charge distribution
>
> The values of AT and AP affect *only* the conversion from r_0 radii to R radii in the definition of potentials in these namelists. If however you adopt the convention that AT is the target mass number and AP the projectile's, then FRESCO can later display the fractional β values corresponding to given deformation lengths. (These are for information only, and do not affect the couplings.)

3.4.2 Second kind of &pot namelist: TYPE>0

KP, TYPE, IT, SHAPE, p1, p2, p3, p4, p5, p6, p0 or

KP, TYPE, IT, SHAPE, p(:) or

KP, TYPE, IT, SHAPE, V,Vr0,Va, W,Wr0,Wa

also**: LSHAPE, JL, XLVARY, ALVARY, DATAFILE**

An empty namelist ends reading potential parameters, as does a negative KP value in the last namelist.

For TYPE

0		Coulomb potential (see 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

9	SHAPE	Effective mass: reduction from unity
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 Tourreil & Sprung (SSC(C))
21	NUM	User-supplied N-N potential via subroutine NNPOT.

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,

SHAPE indicates the radial shape of the form factor,

P1-P3 & P4-P6 are parameters for the real and imaginary parts (respectively).

P0≡P7 can give a further parameter.

   If TYPE < 0, add new potential numerically into previous potential, and use abs(TYPE) instead. This saves space, and is useful if adding components to be deformed by a following namelist with $\leq$ TYPE ≤ 13.

   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 free format from from *Input File 4*, or from **datafile** if specified:
First a comment line,
then (free format) NPOINTS, RSTEP, RFIRST,
followed by NPOINTS potential points for the shape in steps of RSTEP starting at r=RFIRST.
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 external file, as above.

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

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

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

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

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

If SHAPE $\geq$ 30, then use SHAPE-30, and define a *J*- or *L*-dependent potential by a factor defined using **JL, LSHAPE, XLVARY, ALVARY**
so that the potential is multiplied by a form factor depending LSHAPE as

=0 : Woods-Saxon = 1 / (1 + 1/E),
=1 : WS squared = 1 / (1 + 1/E)^2
=2 : Gaussian = exp(-RH^2),
where X=L (for JL='L'), X=J (JL='J'), RH = (X-XLVARY)/ALVARY, and E=exp(-RH).

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

If SHAPE ≥ 20 and < 30, then a J_T/π-dependent potential is defined.
For each subsequent coupled-channels set with total angular momentum J_T, a form factor is read into this potential from *Input file # SHAPE*, reading M = RMATCH/HCM+1 complex numbers in FORMAT(6E12.4) from the file as a random-access, with (M-1)/3+1 lines for each form factor.
For each CC set, form factor number $int(J) + 1$ (for SHAPE ≥ 24) or 1/2 for +/- parity (for SHAPE < 24) is read.

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

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

If SHAPE = 42, then a J-dependent potential is defined: use KP = P(Ji+1) for Ji=0–5, and P0 for Ji$\geq$6, with Ji = int(J).
There need only be one &pot namelist for $40 \leq$ SHAPE≤ 43. The values of TYPE and P2-P7 are ignored. No files are used. Choices are listed in fort.48

Nucleon - nucleon Potentials

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

3.4.3 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 namelist. This preceding namelist must be of TYPE=0 for Coulomb deformations, or TYPE = 1 or 2 for nuclear deformations: deformation of non-central forces is not yet implemented.

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

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

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

Thus, for (possibly hypothetical) $0 \rightarrow k$ transitions, $Mn(Ek) = \langle k||Ek||0\rangle$.
Mn(E2) is related to the intrinsic quadrupole moment in the rotational model by $Mn(Ek) = Q_0 \sqrt{5/16\pi}$. For a uniformly charged sphere of radius R, to first order in β_k we have

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

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

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

$$
\begin{aligned}
M(Ek) &= i^{I-I'+|I-I'|} \langle I'||Ek||I\rangle & (4)\\
&= \pm\sqrt{(2I+1)\,B(Ek,I\to I')}\,, & (5)
\end{aligned}
$$

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

$$
Q_2 = \sqrt{16\pi/5}\,(2I+1)^{-1/2}\,\langle II20|II\rangle\,\langle I||E2||I\rangle\,. \tag{6}
$$

The intrinsic and reduced matrix elements are therefore connected by

$$
M(Ek) = Mn(Ek)\,(-1)^{[I-I'+|I-I'|]/2}\,\sqrt{2I+1}\langle IKk0|I'K\rangle \tag{7}
$$

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 $B(Ek, 0 \to k)$ with some sign within $K = 0$ bands. Mn(Ek) always has the same sign as β.

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 β 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.*

3.4.4 Pairwise couplings

For TYPEs 12–17, namelists **&step** 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.

&step IB,I A, k, STR /

to put in a coupling *to* state IB *from* state IA, of multipolarity k and strength STR. These are terminated by an empty **&step** namelist, or by IB<0 indicating the last entry.

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 $< IB|M(Ek)|IA > = $ M(Ek, IA→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

$$
\begin{aligned}
RDEF(k, I \to I') &= DEF(k)(-1)^{[I-I'+|I-I'|]/2}\sqrt{2I+1}\,\langle IKk0|I'K\rangle & (8)\\
&= M(Ek)*4\pi/[3ZR^{k-1}] & (9)
\end{aligned}
$$

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 *in*dependent of the projection K values read in the &state

namelists. This of course requires making RDEF(k) and M(Ek) dependent on the spins of the excited states, not on any simple model. Note: monopole potentials are included automatically, even if not listed in a **&step** namelist.

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

SHAPE = 0 to 6 : not used
= 7,8,9 : Read from external file, 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

$$F(r) = M(Ek) \, e^2 \, \frac{\sqrt{4\pi}}{(2k+1)} \, r^{-k-1} \tag{10}$$

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 $-1/\sqrt{4\pi}$:

$$F(r) = -DEF(k) \, \frac{1}{\sqrt{4\pi}} \, \frac{dU(r)}{dr} \tag{11}$$

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, **&step** namelists are again 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. Specify values **IB,I A, 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.

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. The SHAPE and P0-P6 parameters on the TYPE=17 &pot namelist are not used.

3.5 &OVERLAP namelists for one- and two-particle form factors

Read in a namelist for each desired particle-nucleus form factor, then an empty namelist.

KN1, KN2, IC1, IC2, IN

>   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.

KIND 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 $\leftarrow$ 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, NN, L, LMAX, SN, IA, JN, IB

>   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.

KBPOT, KRPOT, BE, ISC, NK, ER

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

KRPOT = index KP' of potential with which to multiply this states' wave function for transfer interactions. If zero, use KBPOT. If the binding potential was adjusted for a specific binding energy, then this adjusted potential (not the original) is used for transfers.

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

BOUND STATES:

ISC = 0 to vary the binding energy for fixed potential,
> 0 to vary the TYPE = ISC component of the potential KBPOT by a scaling factor to give binding energy BE.
< 0 to vary the TYPE = ISC component of the potential KBPOT, as above, but **also** to permanently rescale all the varied potential components. This affects all later bound and scattering states using the potential KBPOT.

CONTINUUM BINS:

ISC (default value 2)
= –2: no weighting or normalisation,
= 1, 2 : weight wave functions by $\exp(-i\delta(k))$, so they are real, before integrating over bin width.
= 3, 4 : weight wave functions by $T(k)$* (useful for resonances)
= –1, 1, 3 : normalise wave functions to unity (by usual square norm). **(This option is not recommended, for physics reasons!)**
≥ 10: use additional k factor in the weighting function, with mod(ISC,10) for above choices. Recommended for low-energy bins.

The values ISC>0 give real-valued bins for single-channel states, but not, in general, for coupled-channels bins. In that case, Fresco stores *all* bound and continuum states as complex functions. 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 in the &Fresco namelist).
In general, ISC=2 is recommended (or ISC=4 for resonances), since then the coupled-channels bins will be nearly real. With ISC=–2 (no phase weighting) there will be different results because of different weighting within the bin. Note that all channels within a bin have the same scalar weighting factor.

IPC, NFL

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 abs(NFL).
> 0 : to read a previously-written wave function from file number NFL.
These wave function files contain a comment line, 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 section 7).

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 discussion for the &cfp namelists, 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 &cfp namelist (as &cfp namelists require 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 in the &partition namelists. (If NAM ≥ 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 leastgr NK=$5 \times |NAM|$ integration steps over this range. (These ER and NK override the input values.)

DM Set particle mass specifically, rather than using mass differences.

NK, ER, E Specific values for this continuum bin.

RSMIN, RSMAX If specified, set the overlap form factors to zero outside the interval [RSMIN,RSMAX]

NLAG, PHASE, AUTOWID Parameters for PLUTO with bound or resonant states.

3.5.1 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 & Jn.

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.

3.5.2   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 in the &overlap namelist are given new meanings:

NN → NPAIRS, the number of pair-products to be summed

L → ℓ_{min} , minimum orbital angular momentum ℓ.

LMAX → ℓ_{max} , maximum orbital angular momentum ℓ.

SN → 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 → J_{12} , total angular momentum of the two-particle state outside J_{core}.

KBPOT → T , total Isospin of the 2-nucleon state (0 or 1)s (used to enforce $\ell + S_{12} + T =$ odd)

KRPOT → 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 $u(R) = < u_{12}(r)|U(r,R) >$ is produced, suitable for zero-range two-nucleon transfer calculations.

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

If ISC ≤ 0, use Gaussian quadrature grid, in blocks of 6th-order positions, for the N-N distance RMIN to RNN (&Fresco namelist).
If ISC ≥ 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):
≥ 0 : one-line summary of U(r,R) form factor for each r.
≥ 1 : overall norm and rms radius of total NN state.
≥ 2 : contour plot of the L,ℓ components included.
≥ 3 : contour plot of the $U(r,R) \times$ interaction potential

NFL < 0 : to write two-nucleon wave-function U(r,R) to file number abs(NFL).
> 0 : to read a previously-written wave function from file number NFL. The values of NPAIRS, l_{min}, l_{max}, S_{min} of *the present* run are ignored. Thus NPAIRS can be set to zero.

3.5.3 Namelist &TWONT

This namelist gives the details of the single-particle wave functions and their amplitudes in the sum of pairs.

NT(1:4, :), COEF(:)
   The sum over I of COEF(I) $|(l_1,s_1)j_1,(l_2,s_2)j_2;J_{12},T\rangle$,
      for $(l_1,s_1)j_1$ given by state $u_1(r_1)$ of KN1 = NT(1,I) > 0,
      and $(l_2,s_2)j_2$ given by state $u_2(r_2)$ of KN2 = NT(2,I) > 0,
   is then transformed into the required KIND = 6 format.

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

If NT(3,I) > 0, then the wave functions $u_1(r_1) \times u_2(r_2)$ are further multiplied by $u_3(r)$ (of KN3 = NT(3,I)) before coordinate transformations. Only the radial shape of KN3 is used, not any angular momentum numbers.

If NT(1,I) = −1, then an external form factor is read in from Fortran file number NT(2,I), and processed using the subroutine EXTERN1. At present, this routine is written to read triton wave functions from the Grenoble Faddeev calculations, only reading wave functions, *not* the potential × wavefunction (so for e.g. stripping, only use prior interactions).

If NT(1,I) = −2, then an external form factor is read in from Fortran file number NT(2,I), and processed using the subroutine EXTERN2. At present, this routine is written to read 3-body wave functions from HH calculations, reading wave functions, *as well as* the potential × wavefunction. The 'vrr' file format is assumed, and the breakup (third) vertex function is ignored.

If NT(3,I) < 0, then the I'th component of the pair summation is simply the product of cluster wave functions $u_1(r)u_2(R)$ where u_2 may be KIND = 0 or 1.

NT(4,I) is not used in this version of FRESCO.

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

For all KINDs, the printout also lists:

DZ = derived charge of the bound particle (always positive).

DM = derived mass of the bound particle

K = the wave number of the bound state asymptotically

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

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

D_0 = zero-range stripping strength for transfers from this stare

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

3.6   &COUPLING namelists

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

ICTO, ICFROM ,KIND, IP1,IP2,IP3, P1,P2, , 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.

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

KIND 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

After &coupling namelists for KINDs 2,3,4,5,6,7 (& 8 if IP2>0), spectroscopic amplitudes are read in by means of **&cfp** namelists. 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 &overlap namelists, so amplitudes need only be entered after the namelist 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 namelist will be blank, to indicate no more &cfp namelists are to be read).

For KIND = 1: General Spin Transfer (with local or non-local external form factors on FILE 'INFILE' [default 4]) See section 8 for more details.

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

IP2
= 0 : read in real values (only if IP3 $\geq$ 0)
1 : read in imaginary values (only if IP3 $\geq$ 0)
2 : read in complex values (only if IP3 $\geq$ 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 section 8 (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 lines (until a blank line):

```
Format 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.

For KIND = 2: <u>Electromagnetic one-photon couplings</u> (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 = λ : The multipolarity of the radiation. If $\lambda > 0$, include all multipoles 1,...,λ permitted by parity, whereas if IP1 < 0, include only the multipole λ = 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.

For 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 = 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
≥ 10 : read namelist **&scale** for complex factors [QSCALE(Q), Q=max(0,-IP1):abs(IP1)] to scale the folded form factors for multipoles Q.

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).

For 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 this namelist.

In both KINDs, read in &cfp namelists, 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 the parameter INH in the &Fresco namelist.

For 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 θ quadrature from θ = π down to θ = 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 namelist after this coupling, before any subsequent couplings. This is does not affect the one-step amplitudes, and is only useful if another transfer step follows this coupling.

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

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

P1,P2 : not used.

For KIND = 8: <u>Non-orthogonality supplement</u> 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 &cfp namelists (Only useful if you did NOT have a previous KIND 5, 6 or s7 interaction, which would have needed the amplitudes then.)

$= 0$: no &cfp namelists 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 namelist, then this is double counting.

3.6.1   &CFP namelists

Spectroscopic amplitudes for the overlaps between partitions ICTO & ICFROM already defined by a &coupling namelist:

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 in an &overlap namelist.

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

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

$$(\ell, s)j, J_{core}; J_{com} \tag{12}$$

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 &cfp namelist

If IN=0, no more &cfp namelists to be read.

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

4 Input CDCC format

&CDCC namelist

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

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, Λ_{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),

iscgs,ipcgs = isc,ipc (&overlap) for the projectile ground state wave function,

elab = ELAB(1), just the one projectile lab energy,

hktarg = target value of $h.K$, where h=HCM and K is the elastic wave number. (default hktarg=0.2).

   If HCM=0 in &Fresco namelist, 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 Λ: $\langle KN|\Lambda|KNP \rangle$

= 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 Λ_{max}=la=ip5 are unset, then q sets the maximum multipole order of Λ, 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 = Λ_{max} maximum order for new multipole.

   Note: λ 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 line 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` in a &partition namelist,
`spin,parity` as `Jp/t, Bandp/t` in a &states namelist.
`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 (±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 a &overlap namelist, 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, idef, beta2c, beta3c, beta2m, beta3m`
where this namelist 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 `idef`:

= 0 : Coulomb & nuclear (complex)

= 1 : nuclear (complex) only

= 2 : Coulomb only

Sample CDCC input file:

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

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

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

5 Input SFRESCO format

This is an program which search for a χ^2 minimum when comparing the outputs of FRESCO with sets of data, using the MINUIT search routines.

The inputs for SFRESCO specify the FRESCO input and output files, the number and types of search variables, and the experimental data sets.

5.1 Search file

A `search_file` format is defined as follows:

```
(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:

```
namelist  &variable:
name,kind,step,valmin,valmax, kp,pline,col,potential,nopot,
dataset,datanorm, nafrac,afrac,
energy, jtot,par,channel,width,
```

`name` is name of variable (up to 10 characters),
`kind`: 0=ignore, 1=potential, 2=afrac, 3=R-matrix energy,
  4=R-mat partial width, 5=dataset normalisation
`step`: step size for finding derivatives etc, zero for fixed. (default 0.01)
`valmin`: strict lower bound (if non-zero),
`valmax`: strict upper bound (if non-zero),
`null`: (default -124578) 'undefined' value,

 `kind=`**1: Variable potential parameter:**
`kp`: number of potential as in &pot namelist,
`pline`: order of which &pot namelist within potential definition,
`col`: number within namelist: selecting P0–P7 ,
`potential`: value of this potential parameter (default `null`: use `input_file`)

 `kind=`**2: Variable spectroscopic amplitude:**
`nafrac`: order number of &cfp namelist in `input_file`
`afrac`: spectroscopic amplitude A (default `null`: use `input_file`)

`kind`=**3: Variable energy of R-matrix term:**
`term`: term number (default 1)
`jtot`: J value for additional R-matrix term
`par`: parity (+1 or –1)
`energy`: energy (cm MeV in entrance channel) of additional R-matrix term (default 0)
`nopot`: Disable potential & Buttle correction for this J/pi set (logical T or F, default F)

`kind`=**4: Variable partial width of R-matrix term:**
`channel`: channel number (in order generated by FRESCO)
`term`: term number (default 1)
`width`: width for this channel (MeV$^{1/2}$ 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)

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

```
namelist \&data:
type,data_file,points,delta,xmin,lab,energy,angle,
idir,iscale,abserr,ic,ia,k,q,jtot,par,channel,value,error,   % leg,
pel,exl,labe,lin,lex, % ib % term
```

`type` (default 0)
= 0 angular distribution for fixed energy
= 1 excitation and angular cross section double distributions
= 2 excitation cross section for fixed angle
= 3 excitation total cross section. Also: ic=0: ia=0 is total reaction cross section; `ia`=1 is total fusion cross section; 1<`ia`<NFUS+1 are fusion from potential KFUS (in &Fresco namelist) for inelastic state `ia`–1.
= 4 excitation phase shift for fixed partial wave
= 5 desired factor for bound state search (binding energy or potential scale according to ISC).
= 6 specific experimental constraint on a search parameter `par`, to be `value` with error `error` (`abserr`=T or F).

`data_file`: name of data file with data, '=' for `search_file`, '<' for stdin (default '=')
`points`: number of data points (default: keep reading as many as possible),
`delta`: if non-zero, construct linear x-scale from `xmin` in steps of `delta`, (default 0)
`lab`: T for lab angles and cross sections (default F for cm frame).
`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.

5.2 Sfresco commands

The inputs to `SFresco` are

Card 1: name of `search_file`

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

EX: exit

Q: query status of search variables

SET `var val`: set variable number `var` to value `val`.

FIX `var`: fix variable number `var` (set `step`=0).

STEP `var step`: unfix variable number `var` with step `step`.

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

SHOW: list all datasets with current predictions and χ values.

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

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

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

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

6 Test run: a CCBA calculation

The following test case calculates the inelastic and transfer cross sections for the reactions induced by ^{19}F on ^{28}Si at 60.0 MeV. A Triton-Oxygen cluster structure is assumed for ^{19}F, with the potentials for the triton and the oxygen core being folded together to give a diagonal Watanabe potential for elastic ^{19}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}O + ^{31}P channel, thus performing a CCBA calculation.

```
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/
```

7 File allocations

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

File no.	Format (Fix/Var)	LRECL (bytes)	Access (Seq/Ran)	Routines	Use
89	F			MULTIP	Folded coupling potentials
90	F				Mean elastic optical potential xys
91	F				Mean elastic optical potential for re-reading
105	V		S	FCN	χ^2 progress during fitting
156	F			FR	Jtotal fusion & reaction cross & parity
200	F	80	S	CRISS	Elastic cross section if not fort.201
201-210	F	80	S	CRISS	Cross sections (cf 14) for states 1-10
301	V		S	CDCIN	New Fresco input
302	V		S	CDCIN	New Fresco input (temp)
303	V		S	SFRESCO	Input search file
304	V		S	SFRESCO	Output plot file
305	V		S	CDCIN	New Fresco input from cdcin, col format
306	V		S	SFRESCO/FRXX0	Input Fresco file
307	V		S	SFRESCO/FRXX0	Initial Output Fresco file
308	V		S	SFRESCO/FRXX0	Main Output Fresco file

8 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 ℓ is the orbital angular momentum transfer. These coupled operators are defined following in Bohr & Mottelson, Vol. 1, section 1A-5c, as

$$(F_{\lambda_1}G_{\lambda_2})_{\lambda\mu} = \sum_{\mu_1\mu_2} \langle\lambda_1\mu_1,\lambda_2\mu_2|\lambda\mu\rangle F_{\lambda_1\mu_1}G_{\lambda_2\mu_2} \, , \tag{13}$$

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

$$(F_\lambda G_\lambda)_{00} = (2\lambda+1)^{-1/2}\sum_\mu (-1)^{\lambda-\mu} F_{\lambda\mu}G_{\lambda-\mu} \, . \tag{14}$$

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 FRESCO by:

$$\langle j_f m_f|\hat{O}_{\lambda\mu}|J_i m_i\rangle = (2j_f+1)^{-1/2}\,\langle j_i m_i,\lambda\mu|j_f m_f\rangle\,\langle j_f||\hat{O}_\lambda||j_i\rangle \tag{15}$$

The matrix elements of this operator are

$$\langle (LI_p)J,I_t;J_T M_T|\,\mathbf{S}([\ell,s_p]s_t,s_t)\,|(L'I_p')J',I_t';J_T M_T\rangle$$

$$= (-1)^{s_t+J_T+J'+I_t}\left\{\begin{array}{ccc} J' & I_t' & J_T \\ I_t & J & s_t \end{array}\right\}\hat{J}\hat{J}'\left\{\begin{array}{ccc} L' & I_p' & J' \\ \ell & s_p & s_t \\ L & I_p & J' \end{array}\right\}\frac{1}{\sqrt{4\pi}}\hat{\ell}\hat{L}\langle L0\,\ell0|L'0\rangle$$

$$\times\langle I_p||s_p||I_p'\rangle\langle I_t||s_t||I_t'\rangle \tag{16}$$

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 from data files.

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.

9 Stabilization method for coupled channels solutions

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

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

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

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

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