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

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

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

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

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

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

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

2 Input Cards

```
Card 0:
10A8 HEADNG(10)
```

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

```
Card 1:
10F8.4  HCM,RMATCH,RINTP,HNL,RNL,CENTRE,HNN,RNN,RMIN,RSP
```

Wave functions calculated at intervals of HCM up to abs(RMATCH).
If RMATCH < 0, then read Card 1a for coupled Coulomb wave functions.
Non-local kernels $K'_{fi}(R_f, D_{fi})$ calculated at R_f intervals of RINTP, and for a non-local (D_{fi}) range of RNL centred at CENTRE in steps of HNL. RMATCH and RINTP are rounded to multiples of HCM, and HNL is rounded either to a multiple or a sub-multiple of HCM.
For two-nucleon transfers, the nucleon-nucleon distance is discretised from RMIN to RNN in a multiple of 6 Gaussian quadrature points to give step size approx. HNN.
When folding single-particle states (bound states or continuum bins) with KIND=3 or 4 couplings, the state radii are limited to RSP.

```
Card 1a:
2F8.6, 2F8.2    RASYM,ACCUR,SWITCH,AJSWITCH
```

Use coupled Coulomb wave functions out to asymptotic radius RASYM from inner radius abs(RMATCH) for those partitions in which PWF is TRUE.
If RASYM < 0, then determine the outer radius in order that classical Coulomb trajectories reach an angle abs(RASYM) degrees.
ACCUR is an accuracy parameter controlling the piecewise step length. Default is 0.01: smaller values give greater accuracy.
SWITCH is the radius at which to switch from Airy functions to sines and cosines in piecewise method. Default is 1000 fm.
AJSWITCH - default is 0.0
Normally the Coupled Coulomb wfns are matched to zero and the Numerov integration is omitted, when the Coulomb distance of closest approach is more than 4.5 fm outside abs(RMATCH) (or the -CUTR distance if CUTR negative). This is only allowed when $J_{total} \geq$AJSWITCH.

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

Calculate coupled-channels sets with total J in the interval max(0,JTMIN) $<$ J $<$ JTMAX, stopping sooner if the absorbtion from the elastic channel is less than ABSEND millibarns of three successive J/parity sets. (If ABSEND < 0, this takes the full J interval.)
If JTMIN < 0, then for J $<$ abs(JTMIN) include only the incoming channel in the calculations, ignoring tranfers and excited states. This is needed if the elastic scattering cross sections are to be given correctly.

DRY is normally F (false), but if T (true) the code does a 'dry run' to check that all arrays are of sufficient size. All coupled channel sets are generated, but only the elastic channels should be non-zero.

JSETS = number of coupled-channels sets to be solved, for each energy on Card 19. JSETS = 0, blank or F, for no special limit.
If JSETS = 'P', include only positive parity coupled channels sets,
If JSETS = 'M' or 'N', include only negative parity coupled channels sets.

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

NEARFA
= 0 or 1 for the usual cross sections,
= 2 or -2 for printing 'far side' cross sections too,
= 3 or -3 for printing far and near side cross sections too.
> 0 for printing far & near-sides for elastic channel only.
< 0 for printing far & near-sides for all channels.

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

```
Card 3:
2I1,F6.4,F8.4,F7.4,I1,3F8.4  KQMAX,PP,THMIN,THMAX,THINC,KOORDS,CUTL,CUTR,CUTC
```

Give cross sections (and tensor analysing powers up to rank K = KQMAX) for centre-of-mass scattering angle from THMIN to THMAX in steps of THINC.
Calculate analysing powers/polarisations for projectile (PP=0 or blank), target (PP=1), ejectile (PP=2) or residual nucleus (PP=3).

KOORDS determines the coordinate systems used for the analysing powers:

KOORDS = 0 : Madison coordinates (default)
= 1 : Madison + Transverse
= 2 : Madison + Transverse + Recoil
= 3 : Madison + Transverse + Recoil + Hooton-Johnson

CUTL = radial points per L (angular momentum of partial wave) of lower radial cutoff when integrating the radial equations. Default = -1.6
When CUTL>0, use $\ell = J_{total}$ (total angular momentum of CC set),
When CUTL<0, use $\ell = L_{in}$ (orbital angular momentum of incoming partial wave).
Using CUTL<0 gives more accurate analysing powers.

CUTR = lower radial cutoff (fm). Use max(CUTL*ℓ*HCM,CUTR).
If CUTR < 0, put cutoff at point-Coulomb turning point $-|$CUTR$|$.

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

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

2F8.4     2I2,      2f8.6
ERANGE,DK,INH,plane,smallchan,smallcoup
```

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

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

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

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

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

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

PADE

= 0 for no Pade acceleration,

= 1 for Pade acceleration by the epsilon algorithm,

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

ISO

= 0 or blank, for no isocentrifugal approximations,

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

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

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

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

MAXL,MINL are the maximum and minimum L values for the non-local kernels. If zero, MAXL has the default value JTMAX+6, and if MINL <0 it takes the default value |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 $(30/\mathrm{NNU})^2\%$.

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

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

INH

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

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

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

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

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

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

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

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

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

NUMNODE = number of parallel nodes for PVM operation

If IBLOCK<0, then read:

```
Card 4.5
2i4,           I1,    L2,     I2,  i2,   f6.4, f8.4
NRBASES,NRBMIN,BUTTLE,PRALPHA,PCON,MEIGS,RMATR,EBETA
```

NRBASES = target number of radial basis states in each channel. (Use 2*NRBASES for the elastic and first-inelastic channel for more accuracy).
NRBMIN = minimum number of radial basis states.
BUTTLE = 2 for none, 1 for real, 0 for complex Buttle correction (default 0)
PRALPHA = print basis-state eigenvalues to files fort.60,61,62,63
PCON = trace variable for calculation of radial basis states (same meaning as IPC on Cards 13 for single-particle bound states).
MEIGS = maximum number of bound states to find, if ENLAB < 0 on Card 19.
RMATR = R-matrix matching radius (default is RMATCH on Card 1).
EBETA = energy $\hbar^2 k^2/2m$, where $k = f'/f$, the logarithmic derivative for all radial basis states at r=RMATR, with k having the same sign as EBETA.
If R-matrix solutions are selected (by IBLOCK<0) then all channels are 'blocked' together and solved in a full CRC procedure.

2.1 Trace Control Variables:

```
Card 5 :  14I2
CHANS,LISTCC,TRENEG,CDETR,SMATS,XSTABL,NLPL,WAVES,LAMPL,VEFF,KFUS,WDISK,BPM,MELFIL,CDCC,NFUS
```

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 potentials as they are calculated from Cards 10
- ≥ 3 : Print all potentials as they are calculated from Cards 9

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

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

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

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

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

WDISK

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

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

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

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

The following data formats are used when WDISK > 0 :

```
card A: (I4,2F8.4,F8.1,I3)          NR,H,ENLAB,JTOTAL,PARITY :
                           number radial points, step size, lab. energy,  $J,\pi
card B: (2I4,2F6.1,I4,F6.1,2F15.10)
```

```
IT,L,J,JTOT,LIN,JIN,SMAT (complex)
```

where
IT = index to excited state pair, counts cards 7.
L = partial wave
J = L + projectile spin
JTOT = total spin = J_{total} = J + target spin
LIN = incoming partial wave
JIN = incoming J value.
SMAT = S matrix element for this partial wave.

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

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

BPM

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

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

MELFIL

$= 1$: Write real files 53 and 54 in the 'mel' and 'spec' format for use e.g. by R-matrix program `sturmxx`.

$= 2$: Write complex files 53 and 54 in the 'mel' and 'spec' format.

CDCC

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

```
card A: (F10.4,3F8.4)   ENLAB,Bproj,H2SM,e^2    lab energy,projectile binding energy
                                                hbar^2/2.m, e^2
card B: (4f8.4)         massp,masst,massc,massv masses projectile, target, core, valence
card C: (4f8.4)         Zp,Zt,Zc,Zv             charges
card D: (4A8)           namep,namet,namec,namev names
card E: (4f8.1)         Jp,Jt,Jc,Jv             g.s. spins
card F: (4i8)           Pp,Pt,Pc,Pv             g.s. parities
card G: (4I4)           NBINS,NKMAX,NEXB,NNJMAX no. CDCC bins, max NK,
                                                no. excited states, max(2*Jex+1)
card H: (I4,2f8.4)      NANGL,THMIN,THINC       (cm angular range from Card 3)
for each of the NBINS bins:
 card I:(i2,2f4.1,3f8.4,2i4)
        l,j,Emid,kmin,kmax,NK,KN,ISC
           l,j: quantum numbers  (s==Jv)
           Emid:  centre of bin with respect to continuum threshold
           kmin,kmax,NK: Min,max and number of k values in bin integral
           KN:  original KN index for bin state
           ISC:  normalisation used for bin
    for each IK=1,NK
        card J: (10f8.4) delta(IK): nuclear phase shift used in bin integral (radians)

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

The phase convention 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.

Summary of bin normalisation factors for different ISC values:

ISC

$= 2$: $\exp(-i\delta(k))$

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

$= 12$: $k\exp(-i\delta(k))$

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

2.2 Partitions and Excited States

```
Card 6  (for each partition IC=1,2,... repeat until a blank card 8) :

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

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

Abs(NEX) = number of pairs of excitations of projectile and/or target,
PWF = T, if acceleration of long-range Coulomb couplings to be performed when card 1a present. Default is T.
QVAL = Q value of this partition, relative to the Q-values of the other partitions, for Ep = Et = 0.
If NEX < 0, then cross sections for this partition are not printed.

```
Card 7 (repeat NEX times before the next Card 6) :

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

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

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

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

J = spin of the state

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

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

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

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

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

E = excitation energy of state relative to ground state.

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

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

KP = index of optical potential for this pair of excited states.
PWF= T to use CRCWFN coupled Coulomb wave functions in this partition (see Cards 1,1a)
If zero, use as default KP = IC, the number of this partition.
If EXCH = T calculate and write out all cross sections and amplitudes for $180 - \theta$.
If IGNORE = T, ignore the convergence of this state pair (see IPS discussion on Card 4).
If INFAM $\neq 0$, read in complex amplitudes later to add to calculated scattering amplitudes (see cards A3). (If INFAM < 0, read in only one amplitude (non spin-flip) for each scattering angle.)
If OUTFAM $\neq 0$, write out complex amplitudes later to add to calculated scattering amplitudes (see cards A3). (If OUTFAM < 0, write out only one amplitude (non spin-flip) for each scattering angle: the average of diagonal amplitudes.)

Cards A3 : Extra scattering amplitudes –

If INFAM on a Card 7 is non-zero, then read on file |INFAM|, on a new card for each scattering angle, some complex amplitudes $f(\theta)$, to be added to those calculated by the program before the cross sections are calculated.
If INFAM < 0, then only *one* f(external) is read, and this is used for all the diagonal f(mM:mM), the off-diagonal values being zero.
If INFAM > 0, then all the $f(m'M' : mM)$ are read in.

`Card 8:   Blank card for end of reading partitions.`

2.3 Potentials

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

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

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

All the radii are multiplied by CC, which is updated by a TYPE=0 Card 9 to CC = $A\#1^{1/3} + A\#2^{1/3}$ and by TYPE>0 Cards 10, if P0 > 0, to CC = $P0^{1/3}$
R0C = radius (when multiplied by CC) of charge distribution
AC = diffuseness of charge distribution

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

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

for TYPE

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

Where TYPE indicates type of spin tensor or excitation coupling,
IT is '1' or '3' to make this component included only iteratively,
'2' or '3' to NOT subtract this component in KIND=3,4 single-particle couplings,
the SHAPE indicates the radial shape of the form factor,
and P1-P3 & P4-P6 are parameters for the real and imaginary parts (respectively).

If TYPE < 0, add new potential numerically into previous potential, and use abs(TYPE) instead. This saves space, and is necessary if adding together components to be deformed by a following card $10 \leq$ TYPE ≤ 13.
If KP < 0, this will be the last Card 10. Use abs(KP) below, and omit Card 12.

The SHAPEs for volume potentials (TYPE=1 & 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, central part
7: Read Real
8: Read Imaginary
9: Read Complex

For 'SHAPE's 7-9, immediately read in a comment card, then (free format) NPOINTS, RSTEP, RFIRST, followed by NPOINTS potential points for the shape in steps of RSTEP starting at r=RFIRST, reading card images all from *Input File 4* in free format.
Rescale the real part by P1, the imaginary part by P2, and use radius = P3 * CC for subsequent deformation calculations.
If SHAPE = -7, -8, or -9, rewind file 4 before reading from it.

The SHAPEs for surface potentials (TYPE=2), with R, RH and E as before, are the first derivative forms (normalised to -1 when E=1, if reasonable):
0 : Woods-Saxon = - P1 * 4 * E / (1+E)^2
1 : WS squared = - P1 * 8 * E*E / (1+E)^3
2 : Gaussian = - P1 * 2 * exp(-RH*RH) * RH
3 : Yukawa = - P1 * E * (1 + r/P3) / (r*r)
4 : Exponential = - P1 * E
5 : Reid soft core, spin-orbit part ($\times r$, so TYPE 3 & 4 are correct)
7,8,9 : Read from cards, as above.

The SHAPEs for spin-orbit potentials (TYPE=3 or 4) are the surface (TYPE 2) shapes multiplied by 2.000 / (4 * r * (P3 or P6)). 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.

The SHAPEs for tensor potentials (TYPE=5, 6 & 7), with R, RH and E as before, are the second derivative forms (normalised to unity when E=1, if reasonable):
0 : Woods-Saxon = P1 * 8 * E*(E-1) / (1+E)^3
1 : WS squared = P1 * 4 * E*E / (1+E)^3

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

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

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

so that the potential is multiplied by a form factor:
LSHAPE=0 : Woods-Saxon = 1 / (1 + 1/E),
=1 : WS squared = 1 / (1 + 1/E)^2
=2 : Gaussian = exp(-RH^2),
where X=L (for JL='L'), X=J (JL='J'), RH = (X-XLVARY)/ALVARY, and E=exp(-RH).

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

If SHAPE $\geq$ 20 and $<$ 30, then a J_T/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 set of card images, with (M-1)/3+1 card images for each form factor.
For each CC set, form factor number $int(J_T) + 1$ (for SHAPE $\geq$ 24) or 1/2 for +/- parity (for SHAPE $<$ 24) is read.

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.

Deformations

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

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

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

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

Thus, for (possibly hypothetical) $0 \to k$ 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

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

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

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

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

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

The intrinsic and reduced matrix elements are therefore connected by

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

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

So Mn(Ek) is the square root of $B(Ek, 0 \to k)$ 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.*

For TYPEs 12–17, Cards 11 are read to determine the details of the required couplings between each pair of excited states and of the reorientation terms for each individual state.

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

to put in a coupling *to* state IB *from* state IA, of multipolarity k and strength STR.

For 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

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

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

The SHAPEs for deformed potentials (TYPE=10 to 13) are constructed by:
SHAPE = 0 to 6 : not used (as card gives deformation strengths).

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

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

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

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

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

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

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

11: Nuclear multipoles calculated by numerically deforming the radii of the previous potential, and projecting by Gaussian quadrature onto the required multipoles (those k > 0 for which P(k) is non-zero). For small deformation lengths, these SHAPEs are the same as for SHAPE = 10.

12: Same as SHAPE = 11, except that the monopole k = 0 part of the potential is also recalculated by quadrature. A first order correction is made to the radius to improve volume conservation.

13: Same as SHAPE = 12, except that **no** first order correction is made to the radius to improve volume conservation.

For TYPEs 14–17, Cards 11 are read to determine the details of the required couplings between each pair of excited states and of the reorientation terms for each individual state. Only nuclear couplings are yet implemented.

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

to put in a coupling *to* state IB *from* state IA, of multipolarity —k— and strength STR.
For TYPEs=14–17, the IB and IA can reference any combination of projectile and target

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

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

```
Card 12:   Blank card for end of reading potential parameters.
           (Unless the last KP on card 10 was negative)
```

2.4 One- and Two-Particle Form Factors

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

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

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

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

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

```
Cards 13:
 2I3,     3I2,         I2,  1X,A1,  3I2,      F4.1,I2,F4.1,I2,
 KN1,KN2, IC1,IC2,IN, KIND,   CH1, NN,L,LMAX,SN,IA,JN,IB

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

where

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

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

KIND is the kind of coupling order (0 to 4 for one-particle states, and 6 to 9 for two-particle states) :

- = 0 for (LN,SN) JN couplings $\leftarrow$ 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 = 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 custer (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 = 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.

CONTINUUM BINS:
ISC = 0: no renormalisation (not allowed now: ISC set to 2),
= 1,2 : normalise wave functions by $\exp(-i\delta(k))$, so they are real, before integrating over bin width.
= 3,4 : normalise wave functions by $T(k)^*$ (useful for resonances)
= 1,3 : renormalise wave functions to unity (by usual square norm). **(This option is not recommended, for physics reasons!)**
$\geq$ 10: use additional k factor in normalisation, with mod(ISC,10) for above choices. Recommended for low-energy bins.

IPC = print control for further infomation:

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

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

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

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

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

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

2.4.1 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.

2.4.2 Two-particle KINDs

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

NN $\rightarrow$ NPAIRS, the number of pair-products to be summed
L $\rightarrow$ ℓ_{min} , minimum orbital angular momentum ℓ.
LMAX $\rightarrow$ ℓ_{max} , maximum orbital angular momentum ℓ.
SN $\rightarrow$ S_{min} , minimum sum S_{12} of the two nucleons' intrinsic spins (S_{max} = 1.0 always).
IA, IB give core and composite states, as before.
JN $\rightarrow$ J_{12} , total angular momentum of the two-particle state outside J_{core}.
KBPOT $\rightarrow$ T , total Isospin of the 2-nucleon state (0 or 1)
(used to enforce ℓ + S_{12} + T = odd)
KRPOT $\rightarrow$ KNZR, the KN index to a single-particle state $u_{12}(r)$ of KIND 0 or 1, giving the N-N relative motion in the other participating nucleus (usually in the light ion).
If KNZR > 0, then just the overlap $u(R) =< u_{12}(r)|U(r,R) >$ is produced, suitable for zero-range two-nucleon transfer calculations.
BE $\rightarrow$ EPS , the threshold percentage to define components with square norms sufficiently small to be omitted in the final two-nucleon state.
ISC: If ISC $\leq$ 0, use Gaussian quadrature grid, in blocks of 6th-order positions, for the N-N distance RMIN to RNN (Card 1).
If ISC $\geq$ 1, use uniform grid for the N-N distances. Not so accurate.
If ISC $\neq$ 0, print out numerical values of resulting two-nucleon wavefunction U(r,R).
IPC controls the details printed (along with ISC as just above).
IPC $\geq$ 0 : one-line summary of U(r,R) form factor for each r.
$\geq$ 1 : overall norm and rms radius of total NN state.
$\geq$ 2 : contour plot of the L,ℓ components included.
$\geq$ 3 : contour plot of the $U(r, R)\times$ interaction potential
NFL < 0 : to write two-nucleon wave-function U(r,R) to file number abs(NFL).
> 0 : to read a previously-written wave function from file number NFL. The values of NPAIRS, l_{min}, l_{max}, S_{min} of *the present* run are ignored. Thus NPAIRS can be set to zero.
NPAIRS must be less than or equal to the compilation parameter MPAIR.

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

```
Card 14      3(4I3,                          F8.4)
              (NT1(I),NT2(I),NT3(I),NT4(I), COEF(I)), I=1,NPAIRS
```

The sum over I of COEF(I) $|(l_1, s_1)j_1, (l_2, s_2)j_2; J_{12}, T\rangle$,
for $(l_1, s_1)j_1$ given by state $u_1(r_1)$ of KN1 = NT1(I) > 0,
and $(l_2, s_2)j_2$ given by state $u_2(r_2)$ of KN2 = NT2(I) > 0,
is then transformed into the required KIND = 6 format.
The (r_1, r_2) coordinates become (r, R) coordinates, where r = distance between the two nucleons (angular spin ℓ), and R = distance from the core to their centre of mass (corresponding angular momentum is L_{nn}.

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

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

If NT1(I) = –2, then an external form factor is read in from Fortran file number NT2(I), and processed using the subroutine EXTERN2. At present, this routine is written to read 3-body wave functions from HH calculations, reading wave functions, *as well as* the potential × wavefunction. The 'vrr' file format is assumed, and the breakup (third) vertex function is ignored.

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

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

For KIND = 6, construct components of the form $L_{nn}, ((\ell, (s_1, s_2)S_{12})j_{12}; J_{12}, T\rangle$ 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

2.5 Couplings

`Cards 15-17:`

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

```
Card 15
3I4,                 3I2,           2F8.2,  2F4.1
ICTO,ICFROM,KIND,    IP1,IP2,IP3,   P1,P2,  JMAX,RMX
```

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

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

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

The couplings can be of 8 KINDs:

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

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

KIND = 1 or 2 : <u>Excitation of states of the projectile (1) or target (2).</u>
Generation of couplings between specific states of one of the interacting nuclei, by reading in reduced matrix elements for every pair of coupled states and every multipole and direction of coupling.

IP1 = number of Cards 16 to be read. If IP1 <0, then keep reading cards until IB=0, or until IB<0 indicates that the last card 16 has just been read in.

`Card 16 :  4X,5I4,F8.4    IB,IA,k,NO,KP,A`

where IB = index to excited state fed by coupling IA = index to excited state feeding the coupling k = multipole NO & KP determine the form factor by If NO <0, Read Complex form factor for this multipole k If NO = 0, Read Real form factor for this multipole k to read forms, repeat FORMAT(6E12.4) with card images A2 on Fortran input file 4, for RMATCH/HCM+1 radial points (incl. r=0). If NO > 0 and KP = 0, then choose the NO'th multipole read in for this coupling already.

If NO > 0 and KP > 0, then choose the NO'th component of of potential KP determined from Cards 9 & 10, noting that deformation TYPEs can produce more than one component form factor. Only the radial shape of this component is used, not looking at its associated multipolarity.

A = *reduced* matrix element multiplying the designated form factor, including a contribution analogous to the $(-1)^{[I(IA)-I(IB)+|I(IA)-I(IB)|]/2} \times \sqrt{2I(IA)+1} \times \langle I(IA), K,\ k, 0|I(IB), K\rangle$ that would be needed for rotational couplings, (*except* if it were already included, e.g. if a Coulomb multipole was chosen above by NO,KP > 0, with its M(Ek) factor).

You have several ways of factorising the couplings into form factors and matrix elements, but their product must include (a) the basic radial shape, (b) a strength factor such as a deformation length, and (c) the above Clebsh-Gordon factor.

The SHAPE=10 forms contructed earlier in FRESCO have (a) and (b) included, and the Coulomb SHAPEs also have (c) included via M(Ek).

Note also that these couplings are in addition to couplings induced by any potential multipoles from TYPEs 10-13.

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
= 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 cards 16.5, repeating FORMAT(6E12.4) as required, 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).

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

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

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

KIND = 7 : Finite-range transfers.

IP1 = 0,-2 : POST interaction

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

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

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

IP2 = 0 : no remnant

1 : full real remnant

-1 : full complex remnant

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

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

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

P1,P2 : not used.

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

IP1 = 0 : post

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

IP2

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

= 0 : no cards 17 to read.

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

KIND = 9 : General Spin Transfer (with local or non-local external form factors on FILE 4)

IP1 = 0 : local form factor

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

IP2 = 0 : read in real values (only if IP3 = 0 or 1)

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

= 2 : read in complex values (only if IP3 = 0 or 1)

IP3 = 0 : no scaling factors

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

=-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.

If IP3 = 0 or 1, read FROM FILE 4 the following cards (until a blank card):

```
Card 16.6: F8.0,2F8.4,      I4,  2F4.0,   2I4,   4A8
           FNP ,HNP,FSCALE, LTR, PTR,TTR, IB,IA, COMMENT
```

for FNP = number of radial points (as floating number) HNP = step size 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, repeatedly until sufficient data is read,

```
Card 16.7: 6E12.4 (if IP3=0), or (5E16.7) if IP3=1
```

If IP1 =

0, read local form factor from i=IP3+1 to nint(FNP)

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

```
Cards 17:
```

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

```
Read until IN = 0 or IN < 0:
 4X,4I4,         F8.4
    IN,IB,IA,KN, A
```

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

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

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

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

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

for binding a ℓsj nucleon onto a core of spin J_{core} to form J_{com}.

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

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

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

 3I4,      3I2
 0,PEL,EXL,LAB,LIN,LEX
```

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

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

```
Card 19 :  Projectile Energies
3(F8.4,I8),F8.4) :  (ELAB(i),NLAB(i),i=1,3),ELAB(4)
```

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

2.6 Additional Cards on Fortran input file 4:

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

```
FORMAT(6E12.4)
```

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

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

Appendix I : Namelist input in Fortran 90 version

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

The f90 version reads card sequences as above, but can also read NAMELIST input, which is more flexible in allowable number formats.
After the usual Card 0 with title information, the line

```
Card 1:
NAMELIST
```

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

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

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

&FRESCO namelist

This contains all the variables in Cards 1,1a, 2, 3, 4, 5 and 18 and 19:
`hcm,rmatch,rintp,hnl,rnl,centre,hnn,rnn,rmin, rasym,accrcy,switch,ajswtch,`
`jtmin,jtmax,absend,dry,rela,nearfa,`
`kqmax,pp,thmin,thmax,thinc,koords,cutl,cutr,cutc,`
`nrbases,nrbmin,buttle,pralpha,pcon,meigs,rmatr,ebeta,`
`ips,it0,iter,iblock,pade,iso,nnu,maxl,minl,mtmin,epc,erange,dk,`
`inh,plane,smallchan,smallcoup,`
`chans,listcc,treneg,cdetr,smats,xstabl,nlpl,waves, lampl,veff,kfus,wdisk,bpm,melfil,`
`pel,exl,lab,lin,lex,elab,nlab`
along with new variables `fatal,nosol,nangle,pset,jset,inh,psiren,tmp,masfil,unitmass,finec`.
The new variables are:
`fatal` = T/F, if to stop or not when CRC iterations do not converge (previously ITER>0).
`nosol` = T/F, if not to solve the CRC equations, only construct couplings (previously —ITER—<IT0).
`nangle` = number of additional angle in ANGLE(:) for cross sections. (setting of ANGLE(:) is not yet implemented)
`pset` = -1 or +1, to restrict parity of total CRC set (0 = no restriction) (previously from JSETS).
`jset` = number of CRC sets to calculate before stopping (0 = all sets) (previously from JSETS).
`inh` = 0 : zero-range transfer forms in intervals of HCM exactly (previously a PARAMETER).
= 1 : stored in steps of HCM * (proj. core)/(proj. composite mass)
= 2 : stored in steps of HCM * (targ. core)/(targ. composite mass)
So `inh`=2 corrects for longitudinal recoil during transfers with zero-range projectiles.
`psiren` = T/F, to do simple renormalisation of channel wfs after Pade acceleration
`tmp` = name of directory for temporary files: '/tmp' or '.'

`masfil` = name of file of masses of isotopes (used to find masses and charges from the nuclide name, if read-in MASSes are zero).
`unitmass` = unit (in amu) for MASS values read in. Default = 1.000
`finec` = fine-structure constant: used to determine electrostatic e^2. Default = 137.03599d0.
`jump,jbord` = namelist input jump(1) is stored in jump(2) etc for the program.

&PARTITION namelist

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

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

&STATES namelist

Card 7 information: repeat NEX times before the next `partition` namelist:

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

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

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

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

&POT namelist

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

Individual namelists:

Variables `kp, type, shape, itt, p(1:7)`, where `itt` is a logical variable. The `p(1:7)` is synonymous to the set `p1, p2, p3, p4, p5, p6, P7`, and with the array `def(:)`.
The equivalent to Card 9 is obtained if `shape`=0, then A#1=`p1`, A#2=`p2`, R0C=`p3`, and AC=`p4`.

Combined namelists:

All the following variables may be set independently in the `&pot` namelist

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

so A#1=at,A#2=ap, R0C=rc, and AC=ac etc. All the potentials will have the same shape.
The mnep(k) and mnet(k) are the TYPE=11 and 12 Coulomb reduced matrix elements, and the defp(k) and deft(k) are the TYPE=11 and 12 nuclear deformation lengths. matrix elements, for multipolarity k.
This combined namelist is a pre-processing option only: the FRESCO output will be the same as from individual namelists.

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

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

&STEP namelist

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

&OVERLAP namelist

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

Extra variables keep, dm,nk,er,e are also defined:
keep = T to **not** reset all the variables to zero before reading next namelist.
dm = mass of bound particle, if to override default difference.
nk = number of integration steps to form continuum bin.
er = range of continuum bin (if to override erange).
e : If e≠0, then replace be ← - e.
So be = binding energy, and e = eigenenergy.

&COUPLING namelist

This gives the information previously on Card 15.

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

If(kfrag>0) p1 ← kfrag, and if(kcore>0) p2 ← kcore.

&INEL namelist

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

&CFP namelist

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

&SCALE namelist

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

Mass and charge constants

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

Glossary of Indexing Variables

IC,IC1,IC2 index to mass partitions
IA,IB index to projectile-target pairs of excited states within each partition
KP index to table of potentials, for scattering, binding, and folding
KN index to single-particle bound states
KN1,KN2 two-particle bound states are given for a range (RMIN to RNN) of internucleon separations, and are stored in the MSP table from KN1 to KN2 inclusive.
CP index to the coupling set up

Appendix II : Program Versions

The version described here is a newly revised FRXY.1c version, which includes the search facilities in SFRESCO. Version 1c also changes the format of the potential files in fort.4 and the NFL files for bound states.

Changes in the FRXX versions:

(1) TYPE=17 all-order, TYPE=14-16 second-order calculations, and renumbering of TYPE=8 and 9 potentials. SHAPE≥30 L-dependent potentials.

(2) NAMELIST input format.

(3) Addition of R-matrix expansions for scattering and bound states

(4) Gailitis asymptotic wave functions

(5) EXCH,IGNORE,INFAM,OUTFAM on Card 7, and output files 19, 35 reorganised

It replaces the FRXP.18 version of 1997, which is Fortran90 compatible, and thus also replaces the FRX version of 1993, the FRW versions of April 1992, the FRV versions 1 to 6 up to November 1991, the FVT versions of April and August 1990, the FRT version of June 1989, the FRS version of January 1989, the FRR version of June 1987, the FRQ version of December 1986, the FRP version of January 1986, and the FRO version of December 1984.

Changes in the FRX version :

(1) All REAL*4 and COMPLEX*8 replaced by REAL*8 and COMPLEX*16 respectively. This allows greater exponent range on many computers, and fast storage is more readily available these days.

(2) Parallel computation (in FRXP variant) of distinct $J_{total}\pi$ coupled-channels sets, and also of cross sections to different states. Implemented for iPSC/860 with functions MYNODE(), NUMNODES(), IOMODE(NU), and subroutines SETIOMODE(NU,M) CSEND(IT,BUF,LEN,NODE,IPI) CRECV(IT,BUF,LEN) GSYNC()

(3) Including changes from James Christley that give smoother treatment of high partial waves and Coulomb excitation tails.

(4) Change to the default method of lower radial cutoffs, to avoid generating any unphysical polarisation analysing powers.

(5) Correction to transfer stripping form factors which use the M-dependent method for high L-transfers.

Changes in the FRW version :

(1) Complex bin states (for ISC = 0 or ISC ≥ 10).

Changes in the FRV version :

(1) Coupled Coulomb wavefunctions (using those of James Christley, calculated by piecewise-analytic solutions). Invoked by having RMATCH < 0 on Card 1, and (in that case only) a new card 1a with the necessary control parameters.

(2) Additional PARAMETERs KI, KO, KA and NANGLE.
These are the input file, output file, output cross section file, and number of angles, respectively, and will be used in the searching version (currently under development).

(3) Mn(Ek) is used in place of M(Ek) for TYPE 10 & 11 potentials.

(4) Masses of bound particles corrected for binding energy / c^2 (for states with IN < 0 only).

(5) Format of cross section file LCROSS=16 changed slightly, so that it is an input format for Grtool.

(6) ISOCEN parameter introduced to test isocentrifugal approximations concerning the centrifugal barriers.

(7) Potentials read with SHAPEs 7, 8 and 9 now read a preliminary data line of number of step, increment, and first point position.

Changes in the FVT version :

(1) Input PARAMETER of CRAY replaced by MACH, to give finer control over floating-point limit numbers needed for the target machines.

(2) Incoming energies (Card 25) are now real rather than complex. The Coulomb wave functions are now calculated with (the simpler) COULFG rather than COULCC.

(3) SHAPE = 5 for Reid soft-core potential (Aug 90)
(4) Masses of bound particles corrected for binding energy / c^2 (for bound states only: not bin states).
(5) Better control of iterations, with MIN and MAX iteration counts, and selection of channels to ignore for convergence criterion.

Changes in the FRT version :
(1) New parameter MTMIN on Card 4, controlling high L transfers.
(2) Using 'Enhanced Numerov' of Thorlacius & Cooper (JCP 72(1987) 70) with 5 terms in cosh(sqrt(12T)) expansion, but only for the diagonal potl. This gives greatly improved accuracy if the (diagonal) potentials are nearly constant over a large radial range.
(3) Input KOORDS on Card 3, controlling coordinate systems for tensor observables.
(4) COPYt < 0 allowed on Cards 7, for identical particles.
NB: Identical particles with non-zero spin not yet implemented.
(5) IP3 used for KIND 6 couplings to control the finite range parameters.
(6) SHAPE = 10 to 19 to write out potentials to file 25,
SHAPE ≥ 20 to read in J_T-dependent potentials.
(7) PARAMETERS MAXLNP and NFF no longer required.

Changes in the FRS version :
(1) Single particle form factors always real-valued: ISC must be positive for continuum bins.
(2) Implementation of non-local KIND=9 form factors.
(3) New variable IT for potential cards 10, for iterative solution.
(4) Output of mean $< L >$ and mean square $< L^2 >$ for some cumulative cross sections. Here, L is the J-total for the coupled channels set.
(5) New trace variable BPM, for use of Barrier Penetration Model with the 'weighted local equivalent potentials' generated by the couplings.
(6) The wave functions and potential overlaps for nucleon bound states may be saved on a file by means of parameter NFL, and read in again for subsequent calculations.

Changes in the FRR version :
(1) Heading card (0) ALWAYS read.
(2) New coupling form KIND=9 for arbitrary spin transfers, with external local and/or non-local form factors. (Non-local forms not yet implemented)

Changes in the FRQ version :
(1) Increased control over lower radial limits, with 3 parameters on Card 3.
(2) Calculations now correct for INH non-zero. This enables accurate calculation of zero-range transfers (see coupling KINDs 5 & 6, and see Appendix I).
(3) Input energies on Card 19 can be linear ranges.
(4) Input parameter JSETS on Card 2, to limit number of coupled-channels sets for each energy (useful when looking for resonances).

Changes in the FRP version :
(1) A consistent phase convention is used for the i^L factors. These now *only* appear in the main projectile - target partial waves L, and *not* in any of the discrete nuclear states, whether inelastic excitations or composites of core plus nucleon(s).
(2) The two dimensional form factors for nucleon-nucleon bound states may be saved on a file by means of parameter NFL, and read in again for subsequent calculations.
(3) Fusion analysing powers are calculated, for projectile polarisations.

The FRO release only slightly changed the FRN version of July 1984, which replaced the FRM version with modifications :
(1) Calculation of any tensor analysing power K $<$ KQMAX on Card 3

(2) Changed input of potential deformations, reading in M(Ek) values directly for Coulomb transitions, and with the option of reading 'reduced deformation lengths' for arbitary nuclear transitions. Separate projectile and target deformation lengths are allowed, and also the reading of external multipole form factors.
(3) External form factors and amplitudes are read from Fortran File 4 (rather than from File 5 previously).
(4) Scattering amplitudes, if produced, are written on Fortran File 7.
(5) The multipoles of the non-local form factors K_{fi} are calculated in separate L batches, for each separate pair of initial and final bound states. This increases the cpu times, and also the memory slightly, but much reduces the time waiting for I/O completions.
(6) KIND 1 and 2 couplings have been redefined.
(7) Incoming (and intermediate) energies may be complex (or negative).
(8) The data cards have been renumbered in their descriptions here.
(9) The FRO version allows multipole-scaling cards 16.5, and the SHAPE<0 rewind option for external potentials.

Appendix III : A 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.
The Card types and line numbers added here only for convenience:

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

A namelist version of the above input is:

```
Test run: CCBA calculation 28Si(19F,16O) 31P, cluster form factors.
NAMELIST
 &FRESCO
 hcm=.10 rmatch=25 rintp=0.50  hnl=0.100  rnl=3.
 jtmin=0. jtmax=80 absend=.01 kqmax=1  thmin=0. thmax=60.0  thinc=2.5
 iter=1   iblock=2 nnu=30 chans=1  listcc=2 smats=1 elab=60.0
 /
 &PARTITION
   namep='19-F' massp=19. zp=9 nex=2 namet='28-SI' masst=28 zt=14 /
 &states Jp=0.5   Bandp=+1 Ep=0.0  cpot=1          Jt=0.0   bandt=+1 Et=0.0 /
 &states Jp=2.5   Bandp=+1 Ep=0.2 /

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

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

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

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

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

Appendix IV : FORTRAN file allocations

File no.	Format (Fix/Var)	LRECL (bytes)	Access (Seq/Ran)	Routines	Use
1	V		S	Regular FRESCO input when searching	
2	V		S	Search specification file	
3	V		S	Temporary namelists file	
4	F	80	S	INTER	external KIND=1,2,9 form factors
				POTENT	external potentials
5	F	80	S		standard input
6	V	133	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
15	V		S	FR	local equivalent potent
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
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 Ecm
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
48 #	V	133	S	FR	concurrency log file
49 #	V		S	FR,CRISS	S-matrix elements concurrent→10

File no.	Format (Fix/Var)	LRECL (bytes)	Access (Seq/Ran)	Routines	Use
50 #	V	133	S		tmp standard output concurrent→6
51,52 #	V	133	S		unwanted standard output for node N>0
53	V			WRITEMEL	mel file for sturmx(x)
54	V			WRITESPEC	spec file for sturmx(x)
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
63	F			WRITEMEL	Asymptotic coupling coefficients
64	F			RMATRIX	Coupled eigenstates
65 #	F	NLO*2*8	R	QNN	two-particle multipoles
66	V	NLL*NLO*16	S	INTER	KIND=9 nonlocal formfactor
70	F			RMATRIX	Basis state wfs
71	F	132	S	FR	20 pw phase shifts as Elab functions
88	F			RMATRIX	Bound state wfs
89	F			MULTIP	Folded coupling potentials
90	V		S	FR	average local equivalent potential
93	F			FR	Data for PVM distributions
99	F	80	S	CRISS	input J/L rescaling factors
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

where for MACH=8 we have
= distributed file: distinct file name on each node
@ = shared concurrent file: single file, with writes from each node
For PVM (MACH=7), files 9,10,11, 14 and 19 are required to be on a shared file system.
The use of files 19 and 35 have recently changed.

Appendix V : KIND=9 Spin Transfer Couplings

The definition of the KIND=9 spin transfer couplings is not given in the Computer Physics Reports article, so in versions after March 1998 these are redefined, and new Racah algebra factors included. The old factors can still be obtained by IP3=2.

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.

The matrix elements of this operator are

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

In using KIND=9 couplings, 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. The radial shapes have to be read in using Cards 16.7.

The reduced matrix elements are defined by:

$$< j_f m_f|\hat{O}_{jm}|J_i m_i >= \frac{< j_i m_i\ jm|\ j_f m_f >}{\hat{j}_f} < j_f||\hat{O}_j||j_i > \qquad (1)$$

Appendix VI : Search version SFRESCO

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.
A `search_file` format is defined as follows:

```
Card 1:
(2*string, 2*integer: free format)
input_file, output_file, nvariables, ndatasets
```

`input_file`: name of file (in single quotes) with regular FRESCO input
`output_file`: name of file for the final FRESCO output
`nvariables`: number of search variables
`ndatasets`: number of experimental data sets.

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

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

`name` is name of variable (up to 10 characters),
`kind`: 0=ignore, 1=potential, 2=afrac, 3=R-matrix energy, 4=R-mat total width, 5=R-mat partial width, 6=dataset normalisation
`step`: step size for finding derivatives etc, zero for fixed. (default 0)
`valmin`: strict lower bound (if non-zero),
`valmax`: strict upper bound (if non-zero),
`null`: (default -124578) 'undefined' value,

1: Variable potential parameter:
`kp`: number of potential as on Card 10,
`pline`: order of which Card 10 within potential definition,
`col`: number on Card 10: selecting P0–P7 ,
`potential`: value of this potential parameter (default `null`: use `input_file`)

2: Variable spectroscopic amplitude:
`nafrac`: order number of Cards 17 in `input_file`
`afrac`: spectroscopic amplitude A (default `null`: use `input_file`)

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)

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$^{1/2}$) (default 0)

5: Variable dataset normalisation:
`dataset`: index of which dataset (1 up to `ndatasets`) (default 1)
`datanorm`: search on absolute normalisation of this dataset (default: 1.0)

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

```
Card 3: (namelist: 'data')
type,data_file,points,delta,xmin,lab,energy,angle,
idir,iscale,abserr,ic,ia,k,q,jtot,par,channel
```

`type` (default 0)
= 0 angular distribution for fixed energy
= 1 excitation and angular cross section double distributions
= 2 excitation cross section for fixed angle
= 3 excitation total cross section. Also: ic=0: `ia`=0 is total reaction cross section; `ia`=1 is total fusion cross section; 1<`ia`<NFUS+1 are fusion from potential KFUS (on Card 5) for inelastic state `ia`–1.
= 4 excitation phase shift for fixed partial wave
`data_file`: name of data file with data, '=' for `search_file`, '<' for stdin (default '=')
`points`: number of data points (default: keep reading as many as possible),
`delta`: if non-zero, construct linear x-scale from `xmin` in steps of `delta`, (default 0)
`lab`: T or F for lab angles and cross sections (default F). (T not yet implemented)
`energy`: lab energy for this `type`=0 dataset (default: use `ELAB(1)` from Card 19)
`idir` (default 0)
= 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
`channel`: Channel number of entrance channel in coupled channels set (default 1), for phase shift

Data input (free format):

if `type`=1, read: `energy, angle, value, error`
otherwise:
if `delta`≠0, read: `value, error`
if `delta`=0, read: `x, value, error`

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

`SFresco` Input

The inputs to `SFresco` are
Card 1: name of `search_file`

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

EX: exit
Q: query status of search variables
SET `var val`: set variable number `var` to value `val`.
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: write file `search.plot` for reading by `xmgr, xvgr`.
ESCAN `emin emax estep`: scan lab. energy in incident channel, to give phase shifts in fort.71 and fusion & reaction cross sections in fort.40. This is to look for/at resonances, 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.