

An introduction to fresco with commented examples

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Abstract

In this notes I give a brief introduction to FRESKO, the coupled channels computer code written by I.J. Thompson [5]. In particular, some basic examples to the different types of reactions will be presented and commented. Also, the graphical interface XFRESKO will be presented.

1 Introduction

2 Input file

- **Standard input:** in the original versions of fresco up to frxp.18 (1997) fresco uses input files in formatted fortran style. Then, each line obeys a strict format, in which a certain number of columns are reserved for each variable. Fresco can be downloaded from: <http://www.ph.surrey.ac.uk/~phs1it/>
- **Namelist input:** since version frxx, FRESKO allows input files in fortran namelist style, in which each variable is specified in the format *variable=value*. Thus, the strict formatted style is no longer used in this version. However, to allow backward compatibility, a tool is provided to convert from old style to new style.

- **Graphical input:** the enormous number of variables accepted by FRESKO makes sometimes input files difficult to edit or to interpret, specially to the occasional fresco user. In order to make easier the edition of input files, the graphical front-end XFRESKO [3] can be used. In this interface the variables are organized in a logical way, according to the physics that they describe and a short text description is supplied for most variables. The program is distributed for free, under the GNU license, and can be downloaded from: <http://www.cica.es/aliens/dfamnus/famn/amoro/in>

3 Optical Model (OM)

The simplest calculation that can be performed with FRESKO is the standard OM calculation. Here, the interaction between the projectile and target is described in terms of a complex potential, whose imaginary part accounts for the loss of flux in the elastic channel going to any other channels.

The elastic differential cross section is evaluated through the expression¹

$$\frac{d\sigma}{d\Omega}(\theta) = |f(\theta)|^2, \quad (1)$$

where $f(\theta)$ is the scattering amplitude. The quantity $v|f(\theta)|^2/R^2$ represents the flux of particles elastically scattered by the target at angle θ , with v the asymptotic velocity of the outgoing particles. This is obtained from the asymptotic expression of the scattering wave function:

$$\Psi(\mathbf{K}, \mathbf{R}) \rightarrow e^{i\mathbf{K}\cdot\mathbf{R}} + f(\theta)\frac{e^{iKR}}{R}, \quad (2)$$

where \mathbf{K} denotes the incident linear momentum of the projectile in the center of mass system and \mathbf{R} is the relative coordinate between projectile and target.

This in turn is calculated by solving the Schrödinger equation for the complex potential $U(R)$:

$$\left[\frac{\hbar^2}{2\mu}\nabla^2 + U(R) - E \right] \Psi(\mathbf{K}, \mathbf{R}) = 0 \quad (3)$$

where μ is the reduced mass and E is the energy in the center of mass system: $E = \hbar^2 K^2/2\mu$. This equation has a solution with the form of a plane wave

¹This expression corresponds to the case in which there are no spin-dependent forces.

with relative momentum \mathbf{K} plus outgoing scattered waves:

$$\Psi(\mathbf{K}, \mathbf{R}) = e^{i\mathbf{K}\cdot\mathbf{R}} + \chi^{scat}(\mathbf{K}, \mathbf{R}) \quad (4)$$

where $\chi^{(+)}(\mathbf{K}, \mathbf{R})$ represents the set of scattered waves. Notice that in absence of the target ($U(R) = 0$) there are not such scattered waves and $\Psi(\mathbf{K}, \mathbf{R}) = e^{i\mathbf{K}\cdot\mathbf{R}}$. Commonly, the wave function $\Psi(\mathbf{K}, \mathbf{R})$ is decomposed in partial waves, in order to separate the angular and radial parts:

$$\Psi(\mathbf{K}, \mathbf{R}) = \frac{1}{KR} \sum_L (2L+1) i^L \chi_L(K, R) P_L(\cos\theta), \quad (5)$$

where L is the orbital angular momentum between the projectile and target and θ is the angle between \mathbf{K} and \mathbf{R} .

Replacing this solution into the Schrödinger equation (3) we get the following equation for the radial functions $\chi_L(K, R)$

$$\left[\frac{\hbar^2}{2\mu} \frac{d^2}{dR^2} - \frac{\hbar^2}{2\mu} \frac{L(L+1)}{R^2} - U(R) + E \right] \chi_L(K, R) = 0. \quad (6)$$

Asymptotically, the radial functions behave as

$$\chi_L(K, R) \rightarrow \frac{1}{2} i [H_L(KR)^* - S_L H_L(KR)].$$

Here, we distinguish two cases:

- $U(R)$ is a purely short range potential (i.e., decays faster than $1/R$). In this case $H_L(\rho) \rightarrow \rho h_L^{(+)}(\rho)$, where $h_L^{(+)}$ is a spherical Hankel function of the first kind [1]
- $U(R)$ contains a long range part. In this case, $H_L(\rho)$ are the so called Coulomb wave functions.

The coefficients S_L are the scattering matrix (or S -matrix) elements. They are related to the nuclear phase-shifts, δ_L , by:

$$S_L = e^{2i\delta_L} \quad (7)$$

These are very important quantities as all the information of the effect that the target produces on the scattering wave function (and hence in the

observables) is contained in these coefficients. Hence it is possible to write the all the scattering observables in terms of the S -matrix elements. Notice that in the absence of target $S_L = 1$ for all partial waves. Even in the presence of a point Coulomb interaction, these coefficients remains equal to one, as the Coulomb phase-shifts are already included in the Coulomb wave functions $H_L(KR)$. It is also important to note that, if only real potentials are involved, the S -matrices verify $|S_L| = 1$ and the phase shifts δ_L are real numbers. This expresses the conservation of flux of particles (i.e., the number of scattered particles equals the number of incident particles). On the contrary, if the scattering potential contains an imaginary part, then $|S_L| < 1$ and δ_L become complex numbers. In this case, the outgoing flux of particles is less than the incoming flux, indicating that part of the incident flux leaves the elastic channel and goes to other channels.

Then, the calculation of the elastic cross section involves the following steps:

- Integration of the differential equation (6) for each value of L . The integration is carried out starting from $R = 0$ and solving the differential equation in steps of ΔR up to a certain maximum value R_m .
- For R large enough, the solution (5) obeys the asymptotic form (2). Thus, choosing the value of R_m large enough it is possible to identify the scattering amplitude $f(\theta)$ comparison of (2) and the solution (5) for $R = R_m$.

$$f(\theta) = f_C(\theta) + f'(\theta) ,$$

$$f'(\theta) = \frac{1}{2iK} \sum_L (2L + 1) e^{2i\sigma_L} (S_L - 1) P_L(\cos \theta) . \quad (8)$$

- Finally, the differential elastic cross section is evaluated according to Eq. (1).

It results obvious that the particular choice of ΔR and R_m depends on each particular problem. If only short-ranged potentials are involved (eg. neutron scattering) the value of R_m should be chosen outside of the range of the projectile-target interaction. However, in general $U(R)$ has both Coulomb and nuclear parts. The Coulomb part has a long (“infinite”) range that requires special treatment. Actually, in this case the asymptotic solution of (3) does not behave as planes waves and so expression (2) is not strictly valid. In

particular, plane waves should be replaced by the so called Coulomb functions, which are the solutions of the Schrodinger equation in presence of the Coulomb potential alone. For our purposes, the important point to remind is that in that when long-range interactions are present, the radial equations have to be solved up to larger distances in order to “reach” their asymptotic form.

Concerning the radial step, ΔR , its choice will depend mainly on the diffusiveness of the potentials. Very abrupt or sharp potentials will normally require a smaller step.

Finally, a maximum value of L , denoted (L_{max}) has to be chosen. In principle, the sum in (5) goes to infinity. In practice, convergence of the scattering observables is achieved for finite values of L_{max} . Within a semiclassical picture, the orbital angular momentum can be related to the impact parameter, b , and the incident linear momentum by $Kb \approx L + 1/2$. This means that, for a fixed incident energy, large impact parameters correspond also to large values of the orbital angular momentum. If only short-ranged potentials are present, these values of L do not feel the potential of the target. In presence of the Coulomb potential, these large L values are commonly identified with trajectories that explore uniquely the Coulomb part of the projectile-target interaction.

The parameters discussed above are controlled by the following variables in fresco:

- **rmatch**: Matching radius (R_m in the discussion above)
- **hcm**: Radial step
- **lmax**: Maximum partial wave. Fresco also allows fixing the minimum partial wave, through the variable LMIN. However, in normal calculations this will be set to zero.

In the pure optical model approach only the ground state of the projectile and targets are considered explicitly. Thus, a OM calculation only provides the elastic scattering cross section. The loss of flux effect from the elastic channel to the excluded channels (excitations, rearrangement reactions, etc) is assumed to be included in the imaginary part of the optical potential.

Example 1 : ${}^4\text{He} + {}^{58}\text{Ni}$ at $E_{lab} = 10.7 \text{ MeV}$ As an example we have taken the reaction ${}^4\text{He} + {}^{58}\text{Ni}$ at $E_{lab} = 10.7 \text{ MeV}$. The radial part of the

Schrodinger equation was integrated using an step of HCM=0.1 fm and a matching radius RMATCH=25 fm. A total of JMAX=30 partial waves was used. Looking at the output file, it can be seen that the S -matrix is basically one for partials waves around $J = 30$, indicating the convergence of the sum of partial waves. Notice that the trace variable SMATS has been set to 2, in order to get in the output the S -matrix values. The optical potential used consists of two components:

i) the Coulomb potential, specified by the line:

```
&POT kp=1 type=0 itt=F at=58 rc=1.4 /
```

ii) a volume Woods-Saxon nuclear potential, with both real and imaginary components.

```
&POT kp=1 type=1 itt=F p1=191.5 p2=1.37 p3=0.56 p4=23.5 p5=1.37 p6=0.56
```

The variables p1,p2 and p3 (p4,p5,p6) specify the depth, radius and diffusiveness of the real (imaginary) nuclear potential.

Notice that in this kind of calculations, the *overlap* and *couplings* namelists are left empty.

Example 1: Optical Model calculation

4He + 58Ni elastic scattering $E_{cm}=10$ MeV

NAMELIST

&FRESCO hcm=0.1 rmatch=25.0 rintp=0.5 jtmax=30

absend=-0 dry=F

kqmax=1

thmin=1.00 thmax=180.00 thinc=2.00 it0=1 iblock=1 pralpha=F

rmatr=0.0 beta=0.0 nnu=18 smats=2 xstabl=1 pel=1

exl=1 lab=1 lin=1 lex=1 elab=10.7

fatal=F nosol=F psiren=F /

&PARTITION namep='ALPHA' massp=4 zp=2 namet='58Ni'

masst=58 zt=28 qval=0.0000 pwf=F nex=1 /

&STATES jp=0.0 bandp=1 ep=0.0 cpot=1 jt=0.0

bandt=1 et=0.0 fexch=F /

&partition /

&POT kp=1 type=0 itt=F at=58 rc=1.4 /

&POT kp=1 type=1 itt=F p1=191.5 p2=1.37 p3=0.56

p4=23.5 p5=1.37 p6=0.56 /

&pot /

&overlap /

&coupling /

Output code for fresco input written by xfresco v.0.1

at Sun Jan 13 01:17:29 2002

4 Inelastic excitations: coupled channels method

We consider the scattering of a projectile a by a target A . We denote this partition by the index α , i.e., $\alpha = a + A$. The Hamiltonian of the system is expressed as:

$$H = H_\alpha + K_\alpha + V_\alpha , \quad (9)$$

where K_α is the total kinetic energy, V_α is the projectile-target interaction and H_α is the sum of the internal Hamiltonians, i.e., $H_\alpha = H_a + H_A$.

We assume for simplicity that only one of the nucleus (let's say, a) is excited during the collision and that this nucleus has only one excited state. The model wavefunction will have both elastic and inelastic components. It can be expressed as [4]:

$$\Psi = \phi_\alpha(\mathbf{r})\chi_\alpha(\mathbf{R}) + \phi_{\alpha'}(\mathbf{r})\chi_{\alpha'}(\mathbf{R}), \quad (10)$$

where $\phi_\alpha(\mathbf{r})$ and $\phi_{\alpha'}(\mathbf{r})$ are ground state and excited state wave functions of the nucleus a and, hence, are solutions of the Schrodinger equation with the Hamiltonian H_a :

$$\begin{aligned} H_a\phi_\alpha(\mathbf{r}) &= \epsilon_\alpha\phi_\alpha(\mathbf{r}) \\ H_a\phi_{\alpha'}(\mathbf{r}) &= \epsilon_{\alpha'}\phi_{\alpha'}(\mathbf{r}). \end{aligned} \quad (11)$$

The functions $\chi_\alpha(\mathbf{R})$ and $\chi_{\alpha'}(\mathbf{R})$ describe the relative motion between the projectile and target in the different internal states. The total wavefunction Ψ verifies the Schroedinger equation: $(E - H)\Psi = 0$. By projecting this equation onto the different internal states a set of two equations is obtained:

$$\begin{aligned} (E - \epsilon_\alpha - K_\alpha - U_{\alpha\alpha})\chi_\alpha(\mathbf{R}) &= U_{\alpha\alpha'}\chi_{\alpha'}(\mathbf{R}) \\ (E - \epsilon_{\alpha'} - K_{\alpha'} - U_{\alpha'\alpha'})\chi_{\alpha'}(\mathbf{R}) &= U_{\alpha'\alpha}\chi_\alpha(\mathbf{R}), \end{aligned} \quad (12)$$

where $U_{\alpha\alpha}$ and $U_{\alpha\alpha'}$ are the so called coupling potentials. Thus, for example, $U_{\alpha\alpha'}$ is the potential responsible for the excitation from the initial α state to the final state α' . These potentials are constructed within a certain model, as we will see later. In the coupled channel (CC) approach, the coupled equations (12) are solved *exactly*, to give the functions $\chi_\alpha(\mathbf{R})$ and $\chi_{\alpha'}(\mathbf{R})$.

If the number of states is large, the solution of the coupled equations can be a time consuming task. In many situations, however, some of the excited

states are very weakly coupled to the ground state. For example, referring again to the two channels case, this suggests that the inelastic component of the total wavefunction (10) is going to be a small fraction of the elastic one. This allows to get an approximated solution of the coupled equations by setting to zero the inelastic component in the first equation:

$$\begin{aligned} (E - \epsilon_\alpha - K_\alpha - U_{\alpha\alpha})\chi_\alpha(\mathbf{R}) &\approx 0 \\ (E - \epsilon_{\alpha'} - K_{\alpha'} - U_{\alpha'\alpha'})\chi_{\alpha'}(\mathbf{R}) &= U_{\alpha'\alpha}\chi_\alpha(\mathbf{R}). \end{aligned} \quad (13)$$

Thus, the first equation can readily solved. The resulting function $\chi_\alpha(\mathbf{R})$ is then inserted into the second equation, allowing the calculation of $\chi_{\alpha'}$. This is called 1-step distorted wave distorted wave Born approximation (DWBA). An iterative procedure can be then applied by inserting the calculated $\chi_{\alpha'}$ into the first equation in (12) to get an improved function χ_α . Continuing this procedure, we can get 2-step, 3-step, etc DWBA. When the couplings between channels are weak, the DWBA should approach to the full CC solution. However, when couplings are strong convergence problems can be presented.

As in the pure OM calculation, a separation between the angular and radial parts is made in the set of coupled equations (12). This requires the expansion of the potentials $U_{\alpha\alpha}(\mathbf{R})$ and $U_{\alpha\alpha'}(\mathbf{R})$ in multipoles. For example:

$$U_{\alpha\alpha}(\mathbf{R}) = \sum_{\lambda\mu} U_{\alpha\alpha}^\lambda(R) Y_{\lambda\mu}(\hat{R}) \quad (14)$$

where λ is called multipolarity. In principle the expansion above runs from $\lambda = 0$ to $\lambda = \infty$. However, in practice, only the first few multipoles play a significant role in the scattering process. With the variable IP1 (in the namelist &couplings/) we set the maximum value of λ . The specific form of the coupling potentials depend on the adopted model.

The resolution of the coupled equations (12) is significantly simplified if the distorted wavefunctions are separated into their radial ($f_\alpha(R)$) and angular parts. Thus, inserting the multipole expansion (14) into the coupled set of equations one gets:

$$\begin{aligned} [E_\alpha - T_{\alpha L}(R) - U_\alpha(R)] f_\alpha(R) &= \sum_\lambda U_{\alpha\alpha'}^\lambda(R) f_{\alpha'}(R) \\ [E_{\alpha'} - T_{\alpha' L}(R) - U_{\alpha'}(R)] f_{\alpha'}(R) &= \sum_\lambda U_{\alpha'\alpha}^\lambda(R) f_\alpha(R), \end{aligned} \quad (15)$$

with

$$T_{\alpha L}(R) = -\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2} \right).$$

a) Cluster model:

Some nuclei permit an approximate description of their structure in terms of cluster. This is the case of ${}^7\text{Li}$, which is sometimes modeled as two inert clusters ${}^4\text{He}+{}^3\text{H}$. Other examples are ${}^8\text{B}\rightarrow{}^8\text{B}+n$, ${}^{11}\text{Be}\rightarrow{}^{10}\text{Be}+n$, etc.

For such systems, Coulomb and nuclear excitations can be interpreted and calculated in terms of the interactions of each cluster and the target. For example, consider that the projectile is composed of two fragments, denoted 1 and 2. Then:

$$U_{\alpha\alpha}(\mathbf{R}) = \int d\mathbf{r} \phi_{\alpha}^*(\mathbf{r}) U(\mathbf{r}, \mathbf{R}) \phi_{\alpha}(\mathbf{r}) \quad (16)$$

$$U'_{\alpha\alpha}(\mathbf{R}) = \int d\mathbf{r} \phi_{\alpha}^*(\mathbf{r}) U(\mathbf{r}, \mathbf{R}) \phi_{\alpha'}(\mathbf{r}) \quad (17)$$

where

$$U(\mathbf{r}, \mathbf{R}) = U_1(\mathbf{R}_1) + U_2(\mathbf{R}_2) \quad (18)$$

with

$$\mathbf{R}_1 = \mathbf{R} + \frac{m_2}{m_1 + m_2} \mathbf{r}; \quad \mathbf{R}_2 = \mathbf{R} - \frac{m_1}{m_1 + m_2} \mathbf{r} \quad (19)$$

Previous to the solution of the coupled equations, FRESKO has to evaluate the coupling potentials $U_{\alpha\alpha}$ and $U_{\alpha\alpha'}$. This in turn require the internal wavefunctions $\phi_{\alpha}(\mathbf{r})$ and $\phi_{\alpha'}(\mathbf{r})$.

Example 2: ${}^{19}\text{F} + {}^{28}\text{Si}$ at $E_{lab} = 60 \text{ MeV}$ As an example we consider the reaction ${}^{19}\text{F} + {}^{28}\text{Si}$ at $E_{lab} = 60 \text{ MeV}$. Two states are explicitly considered for the ${}^{19}\text{F}$ nucleus, namely the ground state ($J^{\pi} = 1/2^{+}$) and the first excited state ($J^{\pi} = 5/2^{+}$, $\epsilon = 0.2 \text{ MeV}$), as illustrated schematically in Fig. 2. For shortness, and using our previous notation, these states will be denoted α and α' , respectively. In order to account for the couplings between these states, a triton-oxygen cluster structure is assumed for this nucleus. In this example, these couplings are constructed assuming cluster model. We use from here after the notation:

$$\begin{aligned} {}^{17}\text{F} &\rightarrow {}^{16}\text{O} + {}^3\text{H} \\ \text{composite} &\rightarrow \text{core} + \text{valence} \end{aligned}$$

In order to make fresco know which nuclei are the core and the fragment an extra partition is defined. Then, apart from the $^{17}\text{F} + ^{28}\text{Si}$ partition, a partition with the core nucleus as a projectile is defined, and a target which is the original target (^{28}Si) plus the fragment (^3H). This corresponds to the input line:

```
PARTITION namep='16-0' massp=16 zp=8
namet='31-P' masst=31 zt=15 qval=6.1990 pwf=T nex=1 /
```

The projectile-target interaction is then written as

$$U_{^{19}\text{F}, ^{28}\text{Si}}(\mathbf{r}, \mathbf{R}) = U_{^3\text{H}, ^{28}\text{Si}}(\mathbf{R}_1) + U_{^{16}\text{O}, ^{28}\text{Si}}(\mathbf{R}_2). \quad (20)$$

Notice that the $U_{^3\text{H}, ^{28}\text{Si}}$ and $U_{^{16}\text{O}, ^{28}\text{Si}}$ depend on different coordinates. The $U_{^{19}\text{F}, ^{28}\text{Si}}$ interaction can be written as a function of the internal coordinate between the clusters, \mathbf{r} , and the center of mass coordinate \mathbf{R} . Due to the dependence on the coordinate \mathbf{r} , this potential can produce excitations between the different states of the ^{19}F nucleus.

The relevant information is given in a set of *overlap* namelists. For example, for the ground state wavefunction the following overlap namelist is provided:

```
OVERLAP kn1=1 kind=0 in=1 ic1=1 ic2=2 nn=4 sn=0.5 l=0
j=0.5 kbpot=3 be=11.7300 isc=1 /
```

The meaning of the variables is the following:

- **kn1**: index to label this overlap, as it will be have to be referenced later, in a coupling namelist.
- **kind**: is the kind of coupling order for angular momenta. Typically we will use kind=0.
- **in=1**: to specify that this state corresponds to the projectile (for the target in=2).

- **ic1** and **ic2** specify the partition numbers for the core and the composite nuclei. The order is irrelevant, so in our case we can set $ic1=1$ and $ic2=2$, or $ic1=2$, $ic2=1$.
- **nn, l, jn**: are the quantum numbers for the single-particle state we assume that the triton occupies a $4s_{1/2}$ single-particle state and so: $nn=4$, $\ell=0$ and $j=0.5$.
- **sn**: spin of the fragment, in this case, the triton.
- **kbpot**: index of the potential that binds the fragment (triton) to the core (oxygen).
- **be**: binding energy of the triton in the ^{19}F nucleus.
- **isc**: the *type=isc* part of the potential *kbpot* is varied in order to reproduce the binding energy. In this example $isc=1$, and so the depth of the nuclear potential is taken as a free parameter.

An analogous overlap namelist is used for the overlap corresponding to the excited state.

Finally, in order to set up the coupled equations it is necessary to specify the couplings between the different channels. In this example, we have to *tell* FRESKO that we want to couple the ground and excited state in the ^{19}F nucleus. This is done with the namelist:

```
COUPLING icto=1 icfrom=2 kind=3 ip1=4 ip2=1 p1=6.0 p2=5.0/
```

The meaning of the variables is the following:

- **icto**: index of the partition containing the composite nucleus (^{19}F).
- **icfrom**: index of the partition containing the core nucleus (^{16}O).
- **kind**: the flexibility of FRESKO allows many types of couplings: single-particle excitations, zero-range transfer, finite-range transfer, collective excitations,... With the variable *kind* we specify the type of coupling. In our example, it corresponds to single-particle excitation of the projectile ($kind=3$).

- **ip1**: IP1=4 means that the multipoles $\lambda = 0, \dots, 4$ will be considered.
- **ip2**: to specify if the coupling potentials $U_{\alpha\alpha}$ and $U_{\alpha\alpha'}$ will include only the nuclear potential (IP2=1), the Coulomb (IP2=2) or both (IP2=0). In our example, IP2=1, and thus only the nuclear part of the potentials $U(^3\text{H}, ^{28}\text{Si})$ and $U(^{16}\text{O}, ^{28}\text{Si})$ will be considered to construct the folding potentials. This does NOT mean that the Coulomb potential is ignored in the calculation, as the potential KP=1 contains the monopole central potential between the projectile and the target. Thus, with IP2=1 we just suppress excitations between the states α and α' due to the Coulomb interaction.
- **p1**: potential index KP for the valence-target interaction. In our example, this is a (complex) optical potential describing the $^3\text{H} + ^{28}\text{Si}$ elastic scattering.
- **p2**: potential index KP for the core-target interaction. In our example, this is the optical potential $U(^{16}\text{O}, ^{28}\text{Si})$.

Finally, it is necessary to explicitly defined the couplings between different states. This permits a great flexibility as one can check the effect of specific couplings, or omit those couplings that will have very small effect, thus saving computational time.

```
&CFP in=1 ib=1 ia=1 kn=1 a=1.000 /
```

```
&CFP in=1 ib=2 ia=1 kn=2 a=1.000 /
```

The first line gives the amplitude for the overlap $\langle ^{19}\text{F} | ^{16}\text{O} \rangle$, with ^{19}F in its ground state. The second line is for the $\langle ^{19}\text{F}^* | ^{16}\text{O} \rangle$ overlap, with ^{19}F in its excited state (see section 5).

The meaning of the variables for the first line is:

- **in**: to indicate that the overlap is for the projectile (in=1) or target (in=2)
- **ib**: index of state within the projectile that contains the projectile. In this example, the composite is ^{19}F , which appears in partition 1. The ground state appears in the first state defined within this partition and so IB=1.

- **ia**: index of excitation state of core nucleus. In our case, only one state is specified for the core and so IA=1.
- **kn**: is the index of the form factor that provides the wave function for the overlap $\langle {}^{19}\text{F}|{}^{16}\text{O}\rangle$.
- **a**: Is the spectroscopic amplitude for the overlap. In other words, it is the single-particle fraction. In our example, we consider pure single-particle states, and so A=1.

There are also several important variables within the FRESKO namelist which control the way in which the set of coupled equations are solved:

- **iblock**: Is the number of states (starting from partition 1) that will be coupled exactly. In this example we want to couple the two states of the ${}^{19}\text{F}$ nucleus and thus IBLOCK=2.
- **it0, iter**: When the variable IBLOCK is less than the number of states, FRESKO interprets that the rest of states that will not be solved exactly, will be included by iterations. For these states, the number of minimum and maximum iterations are controlled by means of the variables IT0 and ITER. The former is the minimum number of DWBA steps that will be carried out. After IT0 steps FRESKO checks the difference between successive S-matrix elements and compares with the variable IPS. If the difference is smaller than IPS percent, the calculation finished. If not, it continues the iterations up to a maximum of IT0 iterations.

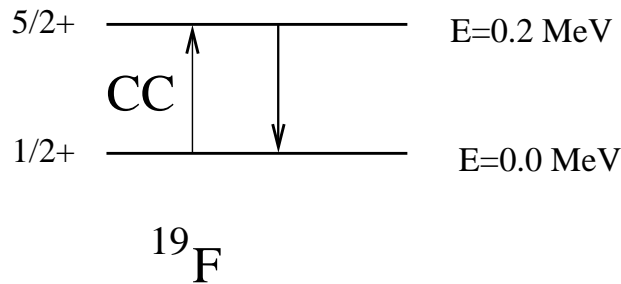


Figure 1: Energy levels for the ^{19}F considered in the CC calculation.

Example 2: CC with cluster form factors

Test run: CC calculation $^{19}\text{F}+^{28}\text{Si}$. Cluster form factors

NAMELIST

```
&FRESKO hcm=0.100 rmatch=25.000 rintp=0.50
hnl=0.100 rnl=3.00 centre=0.00 jtmin=0.0 jtmax=80.0
absend=0.0100 dry=F thmin=0.00 thmax=60.00
thinc=2.50 ips=0.0000 iter=1 iblock=2 pralpha=F
nnu=30 chans=1 listcc=2 smats=1 pel=1 exl=1
lab=1 lin=1 lex=1 elab=60.0
fatal=T nosol=F psiren=F unitmass=1.007335
finec=137.03599 /
```

```
&PARTITION namep='19-F' massp=19 zp=9 namet='28-SI'
masst=28 zt=14 qval=0.0000 pwf=T nex=2 /
&STATES jp=0.5 bandp=1 ep=0.0000 cpot=1 jt=0.0
bandt=1 et=0.0000 fexch=F /
&STATES jp=2.5 bandp=1 ep=0.2000 jt=0.0 et=0.0000
fexch=F /
```

```
&PARTITION namep='16-0' massp=16 zp=8 namet='31-P'
masst=31 zt=15 qval=6.1990 pwf=T nex=1 /
&STATES jp=0.0 bandp=1 ep=0.0000 jt=0.5 bandt=1
et=0.0000 fexch=F /
&partition /
```

```
&POT kp=1 itt=F ap=28.000 at=19.000 rc=1.200 /
```

```

&POT kp=2 itt=F ap=31.000 at=16.000 rc=1.350 /
&POT kp=2 type=1 itt=F p1=31.200 p2=1.450
p3=0.470 p4=15.100 p5=1.270 p6=0.310 p7=0.000 /
&POT kp=2 type=3 itt=F p1=0.750 p2=1.240 p3=0.370 /
&POT kp=3 itt=F ap=19.000 at=0.000 rc=1.250
ac=0.650 /
&POT kp=3 type=1 itt=F p1=115.000 p2=1.250
p3=0.650 /
&POT kp=3 type=3 itt=F p1=6.300 p2=1.250 p3=0.650 /
&POT kp=4 itt=F ap=31.000 at=0.000 rc=1.250
ac=0.650 /
&POT kp=4 type=1 itt=F p1=99.000 p2=1.250
p3=0.650 /
&POT kp=4 type=3 itt=F p1=6.300 p2=1.250 p3=0.650 /
&POT kp=5 itt=F ap=28.000 at=0.000 rc=1.200 /
&POT kp=5 type=1 itt=F p1=27.000 p2=2.425
p3=0.460 p4=11.660 p5=2.145 p6=0.238 p7=0.000 /
&POT kp=6 itt=F ap=28.000 at=0.000 rc=1.250
ac=0.650 /
&POT kp=6 type=1 itt=F p1=160.000 p2=1.070
p3=0.720 p4=37.000 p5=1.350 p6=0.880 p7=0.000 /
&pot /

&OVERLAP kn1=1 ic1=1 ic2=2 in=1 nn=4 sn=0.5 j=0.5
kbpot=3 be=11.7300 isc=1 nam=1 ampl=1.0000 /
&OVERLAP kn1=2 ic1=1 ic2=2 in=1 nn=3 l=2 sn=0.5
j=2.5 kbpot=3 be=11.5300 isc=1 nam=1 ampl=1.0000 /
&overlap /

&COUPLING icto=1 icfrom=2 kind=3 ip1=4 ip2=1
p1=6.0000 p2=5.0000 jmax=0.00 rmax=0.0 /
&CFP in=1 ib=1 ia=1 kn=1 a=1.000 /
&CFP in=1 ib=2 ia=1 kn=2 a=1.000 /
&cfp /

&coupling /

```


b) Collective model:

Within a collective model (eg., vibrational, rotational,...) excitations are interpreted in terms of the deformation of the charge or mass distribution of the nucleus.

In the previous example, the coupling terms $U_{\alpha\alpha'}$ appearing in the coupled equations (12) are determined within a cluster model. In some systems, the excitation spectrum is better described within a collective model. The excitation of the nucleus is then described in terms of deformed potentials. These can be expressed as a change in the radius at which we evaluate the optical potentials, the change depending on the relative orientations of the radius vector to the intrinsic orientation of the nucleus.

Coulomb deformation: The Coulomb potential between a charge Z and a distribution of charges z_i is

$$V_C(\mathbf{r}, \xi) = \sum_i \frac{Z z_i}{|\mathbf{r} - \mathbf{r}_i|},$$

with $\xi = \{\mathbf{r}_i\}$

Again, this potential is expanded in multipoles, resulting

$$V_C^{\lambda\mu}(R, \xi) = M(E_{\lambda\mu}) \frac{\sqrt{4\pi} e^2}{2\lambda + 1} \frac{Z}{R^{\lambda+1}},$$

where

$$M(E_{\lambda\mu}) = \sum_i z_i r_i^\lambda Y_{\lambda\mu}(\hat{r}_i)$$

is the multipole electric operator.

In this scheme, the coupling potentials U_{ij} are the matrix elements of the operator $V_C^{\lambda\mu}(R)$ between different excited states. In the collective model, these states are characterized by their angular momentum I and projection M . Using the Wigner-Eckart theorem

$$\langle I'M' | V_C^{\lambda\mu} | IM \rangle = (2I' + 1)^{1/2} \langle IM \lambda \mu | I'M' \rangle \langle I' || V_C^\lambda || I \rangle, \quad (21)$$

where $\langle IM \lambda \mu | I'M' \rangle$ is just a Clebsch-Gordan coefficient and $\langle I' || V_C^\lambda || I \rangle$ is the so called *reduced matrix element* for the operator V_C^λ . These are given by:

$$\langle I' || V_C^\lambda(R) || I \rangle = \langle I || M(E_\lambda) || I \rangle \frac{\sqrt{4\pi}e^2 Z}{2\lambda + 1} \begin{cases} R^\lambda / R_c^{2\lambda+1} & (R \leq R_c) \\ 1/R^{\lambda+1} & (R > R_c) \end{cases} \quad (22)$$

The evaluation of $\langle I' || M(E_{\lambda\mu}) || I \rangle$ depends on the model used. We consider two cases:

- **Rotational model:**

$$\langle I' || M(E_\lambda) || I \rangle = \sqrt{2I + 1} \langle IK\lambda 0 | I'K \rangle \langle \chi | M(E_{\lambda 0}) | \chi \rangle, \quad (23)$$

where K is the rotational band and $\langle \chi | M(E_{\lambda 0}) | \chi \rangle \equiv M_n(E_\lambda)$ is the expected value of the electric operator $M(E_{\lambda 0})$ in the intrinsic state of the deformed nucleus. The only information required by FRESCO are the expectation values $\langle \chi | M(E_{\lambda 0}) | \chi \rangle$, which are assigned to the variables $P(\lambda)$:

$$P(\lambda) = \langle \chi | M(E_{\lambda 0}) | \chi \rangle \quad (24)$$

- **Experimentally**, $\langle I' || M(E_{\lambda\mu}) || I \rangle$ can be directly related to the reduced transition probability $B(E_\lambda; I \rightarrow I')$:

$$B(E_\lambda; I \rightarrow I') = \frac{1}{2I + 1} |\langle I' || M(E_\lambda) || I \rangle|^2, \quad (25)$$

for the off-diagonal matrix elements. For quadrupole deformations, the diagonal matrix elements are related to the experimental quadrupole moment by:

$$Q_2 = \sqrt{\frac{16\pi}{5}} (2I + 1)^{-1/2} \langle II20 | II \rangle \langle I || M(E_2) || I \rangle, \quad (26)$$

for the diagonal reduced matrix elements. Each matrix element is provided in a separated `&step/` namelist.

- **ib**: final state with angular momentum I'
- **ia**: initial state with angular momentum I
- **k**: multipolarity λ
- **str**: strength of the coupling factor

$$STR = M(E_\lambda) = (-1)^{\frac{I-I'+|I-I'|}{2}} \langle I' || M(E_\lambda) || I \rangle = \pm \sqrt{(2I + 1)B(E_\lambda; I \rightarrow I')} \quad (27)$$

Coupling	TYPE	P(k)	STR
Coulomb: rotational	10,11	$M_n(k)$	-
Coulomb: general	12,13	$M_n(k)$	$M(Ek) = (-1)^{\frac{I-I'+ I-I' }{2}} \langle I' M(Ek) I \rangle$
Nuclear: rotational	10,11	$DEF(k) = R\beta_k$	-
Nuclear: general	12,13	$DEF(k) = R\beta_k$	$RDEF(k) = (-1)^{\frac{I-I'+ I-I' }{2}} \langle I' \delta_k I \rangle$

Table 1: Information required by FRESKO to construct the coupling potentials in a CC calculation

Nuclear deformation: If $U(R)$ is the potential shape to be deformed, the deformed nuclear potential can be constructed as

$$\mathbf{V}(\xi, \mathbf{R}) = U(R - \delta(\hat{R}')), \quad (28)$$

where \hat{R}' are the angular coordinates (θ, φ) referred to the intrinsic reference frame. The function δ is normally expanded in multipoles:

$$\delta(\hat{R}') = \sum_{\lambda} \delta_{\lambda} Y_{\lambda 0}(\hat{R}') \quad (29)$$

As in the case of cluster form factors, it is convenient to expand the coupling potential \mathbf{V} in spherical harmonics, giving rise to the radial multipoles $V_N^{\lambda}(R)$, whose reduced matrix elements are given by

$$\langle I' || V_N^{\lambda}(R) || I \rangle = -\frac{\langle I' || \delta_{\lambda} || I \rangle}{\sqrt{4\pi}} \frac{dU(R)}{dR}, \quad (30)$$

with the same shape for all nuclear multipoles $\lambda > 0$.

The values of $\langle I' || \delta_{\lambda} || I \rangle$ are model dependent:

- **Rotational model:**

$$\langle I' || \delta_{\lambda} || I \rangle = \sqrt{2I+1} \langle IK\lambda 0 | I'K \rangle \langle \chi | \delta_{\lambda} | \chi \rangle, \quad (31)$$

where K is the projection of the angular momenta I and I' within a rotational model and $\langle \chi | \delta_{\lambda} | \chi \rangle$ is the expectation value of the operator $\hat{\delta}_{\lambda}$ in the internal state of the deformed nucleus. Even more, if the mass and charge distributions coincide:

$$\langle I' || \delta_{\lambda} || I \rangle = \frac{4\pi}{3ZeR_0^{\lambda-1}} \langle I' || M(E_{\lambda}) || I \rangle, \quad (32)$$

where R_0 is an average radius. According to (23) and (31) and the previous relation holds also for the matrix elements in the intrinsic state:

$$\langle \chi | \delta_\lambda | \chi \rangle = \frac{4\pi}{3ZeR_0^{\lambda-1}} \langle \chi | M(E_\lambda) | \chi \rangle, \quad (33)$$

In the rotational model, it is not necessary to provide FRESKO with the all matrix elements above. The only information required by FRESKO are the deformation lengths δ_λ , which are assigned to the variables $P(\lambda)$:

$$P(\lambda) = \langle \chi | \delta_\lambda | \chi \rangle = R_0 \beta_\lambda, \quad (34)$$

where β_λ the deformation parameters. Note that within the rotational model, the nuclear and coulomb matrix elements are related by:

$$M_n(E_\lambda) = \frac{3Z\beta_\lambda R^\lambda}{4\pi} \quad (35)$$

- **General case:** In general, if we are not within a specific model, there is not a simple relation between the matrix elements connecting different states I and I' and so it is necessary to give them explicitly for each pair of excited states. In particular, FRESKO uses the matrix elements:

$$\begin{aligned} RDEF(\lambda; I \rightarrow I') &= (-1)^{\frac{I-I'+|I-I'|}{2}} \langle I' | \delta_\lambda | I \rangle \\ &= (-1)^{\frac{I-I'+|I-I'|}{2}} \sqrt{2I+1} \langle IK\lambda 0 | I'K \rangle \langle \chi | \delta_\lambda | \chi \rangle \\ &= (-1)^{\frac{I-I'+|I-I'|}{2}} \sqrt{2I+1} \langle IK\lambda 0 | I'K \rangle \beta_\lambda R_0 \end{aligned} \quad (36)$$

This information is provided to fresco through the namelist **&step/**, which contains the variables²:

- **ib:** final state with angular momentum I'
- **ia:** initial state with angular momentum I
- **k:** multipolarity λ
- **str:** strength of the coupling factor $RDEF(\lambda; I \rightarrow I')$

²In the f77 version, this information is given by means of cards 11.

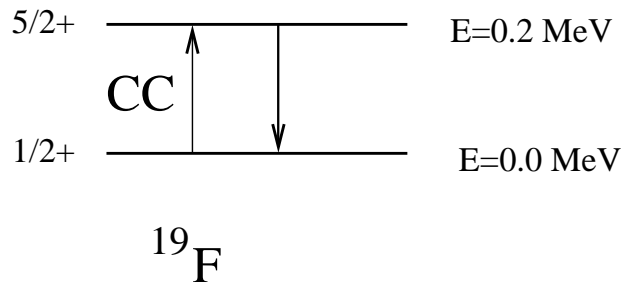


Figure 2: Energy levels for the ^{19}F considered in the CC calculation.

Notes:

- Inclusion of $I \rightarrow I'$ transition in the table of couplings, does not include automatically $I' \rightarrow I$. We then need two `&step/` namelist in order both couplings are considered.
- The values of $M(Ek)$ must be entered in units of $e fm^\lambda$. This means that the reduced transition probabilities, $B(E\lambda)$ are in units of $e^2 fm^{2\lambda}$. Notice that some databases use different units. For instance, the ENSDF database at NNDC [2] uses for the transition probabilities the units $e^2 b^\lambda$. Frequently, transition probabilities are given in Weisskopf units, which are estimates of transition strengths for a single proton in a uniform charge distribution 2.
- The transition probability for an electric radiation is roughly two orders of magnitude larger than for an equivalent magnetic transition, meaning electric transitions are favored, $\frac{\lambda(M1)}{\lambda(E1)} \ll 1$. The probability is also inversely proportional to the multipolarity meaning higher multiplicities are slower, $\frac{\lambda(l+1)}{\lambda(l)} \ll 1$. The effect of this is that while an E2 transition can compete with an M1, the M3 and higher orders are negligible. Also, an M2 cannot compete with an E1, which is therefore generally described as a ‘pure’ dipole.
- Fresco gives also the possibility of defining the couplings to excited states through the `&coupling/` and `&inel/` namelists. As an example, consider the reaction $^8\text{Li} + ^{208}\text{Pb}$ in a two state model of ^8Li , including the g.s. (2^+) and its excited state (1^+). Using the values

Transition rate	Weisskopf estimate
T(E1)=1.587 10 ¹⁵ E ³ B(E1)	B(E1)=6.446 10 ⁻² A ^{2/3}
T(E2)=1.223 10 ⁹ E ⁵ B(E2)	B(E2)=5.940 10 ⁻² A ^{4/3}
T(E3)=5.69810 ² E ⁷ B(E3)	B(E3)=5.940 10 ⁻² A ²
T(E4)=1.694 10 ⁻⁴ E ⁻⁹ B(E4)	B(E4)=6.285 10 ⁻² A ^{8/3}
T(E5)=3.451 10 ⁻¹¹ E ¹¹ B(E5)	B(E5)=6.928 10 ⁻² A ^{10/3}
T(M1)=1.779 10 ¹³ E ³ B(M1)	B(M1)=6.446
T(M2)=1.371 10 ⁷ E ⁵ B(M2)	B(M2)=1.650 A ^{2/3}
T(M3)=6.387 E ⁷ B(M3)	B(M3)=1.650 A ^{4/3}
T(M4)=1.89910 ⁻⁶ E ⁹ B(M4)	B(M4)=1.746 A ²
T(M5)=3.868 10 ⁻¹³ E ¹¹ B(M5)	B(M5)=1.924 A ^{8/3}

Table 2: Transition probabilities T(sec-1) expressed by B(EL) in $e^2 fm^{2\lambda}$ and B(ML) in $(\frac{e\hbar}{2mc})^2 fm^{2\lambda-2}$. E= Gamma-ray energy, measured in MeV.

$B(E2; 2^+ \rightarrow 1^+) = 30 e^2 fm^4$ and the deformation length $\delta = 1.75$ fm from the literature the fresco input looks like:

8Li+208Pb quasielastic

NAMELIST

```
&FRESKO hcm=0.1 rmatch=100 rintp=0.5 hnl=0.033
rnl=3.00 centre=0.00 jtmax=100 absend=0.001 dry=F
jump(1:6:1)=0 0 0 0 0 0 jbord(1:6)=0 0 0 0 0.0 0.0
thmin=2.00 thmax=-180.00 thinc=2.00 ips=0.01 iblock=2
pralpha=F pade=1 nnu=24 chans=1 smats=2 xstabl=1
pel=1 exl=1 lab=1 lin=1 lex=1 elab=34.404
nlab(1:3)=0 0 0 fatal=F nosol=F psiren=T
unitmass=1.000 finec=137.03599d0 /
```

```
&PARTITION namep='Li-8' massp=8 zp=3 namet='Pb-208'
masst=207.977 zt=82 qval=0.0000 pwf=T nex=2 /
&STATES jp=2.0 bandp=1 ep=0.000 kkp=1 cpot=1
jt=0.0 bandt=1 et=0.000 fexch=F /
&STATES jp=1.0 bandp=1 ep=0.981 kkp=1 cpot=1
jt=0.0 copyt=1 bandt=1 et=0.000 fexch=F /
```

```
&partition /
```

```

&POT kp=1 itt=F ap=8 at=208 rc=1.200 /
&POT kp=1 type=12 shape=10 itt=F p1=0.000 p2=10.
p3=0.000 p4=0.000 p5=0.000 p6=0.000 /
&STEP ib=2 ia=1 k=2 str=12.24 /
&STEP ib=1 ia=2 k=2 str=12.24 /
&STEP ib=1 ia=1 k=2 str=-5.976 /
&STEP ib=2 ia=2 k=2 str=5.477 /
&step /

```

```

&POT kp=1 type=1 itt=F p1=60 p2=1.3 p3=0.65
p4=150 p5=1.3 p6=0.60 /
&POT kp=1 type=12 shape=10 itt=F p1=0.000 p2=1.75
p3=0.000 p4=0.000 p5=0.000 p6=0.000 /
&STEP ib=2 ia=1 k=2 str=2.1433 /
&STEP ib=1 ia=2 k=2 str=2.1433 /
&STEP ib=1 ia=1 k=2 str=-1.0458 /
&STEP ib=2 ia=2 k=2 str=0.9585 /
&step /

```

```

&pot /

```

```

&overlap /

```

```

&coupling /

```

Output code for fresco input written by xfresco v.1.0
at Mon Sep 23 16:03:22 2002

Alternatively, we can define a `&coupling/` namelist with `kind=1` (excitations of projectile):

```

\&COUPLING icto=1 icfrom=1 kind=1 ip1=8 /

```

Here, `icto=icfrom` indicates the partition where excitations are defined. Then, a `&inel/` namelist is included for each coupling. For instance,

```

&INEL ib=2 ia=1 k=2 no=2 kp=1 a=12.24 /

```

that state $ia=1$ (i.e., the g.s.) is coupled to state $ib=2$ (the excited state) with multipolarity $k=2$. The coupling will be generated using the component $no=2$ of potential $kp=1$ (which corresponds to a deformed coulomb potential). Note that this amplitude a is to be multiplied to the value of $p(k)$ in the deformed potential. The product of both quantities is supposed to give the reduced matrix element $M(Ek; I \rightarrow I')$ (for Coulomb couplings) or $RDEF(k; I \rightarrow I')$ (for nuclear couplings)

8Li+208Pb quasielastic

NAMELIST

```
&FRESKO hcm=0.1 rmatch=100 rintp=0.5 hnl=0.033
rnl=3.00 centre=0.00 jtmax=100 absend=0.001 dry=F
jump(1:6:1)=0 0 0 0 0 0 jbord(1:6)=0 0 0 0 0.0 0.0
thmin=2.00 thmax=-180.00 thinc=2.00 ips=0.01 iblock=2
pralpha=F pade=1 nnu=24 chans=1 smats=2 xstabl=1
pel=1 exl=1 lab=1 lin=1 lex=1 elab=34.404
nlab(1:3)=0 0 0 fatal=F nosol=F psiren=F
unitmass=1.000 finec=137.03599d0 /
```

```
&PARTITION namep='Li-8' massp=8 zp=3 namet='Pb-208'
masst=207.977 zt=82 qval=0.0000 pwf=T nex=2 /
&STATES jp=2.0 bandp=1 ep=0.000 kkp=1 cpot=1
jt=0.0 bandt=1 et=0.000 fexch=F /
&STATES jp=1.0 bandp=1 ep=0.981 kkp=1 cpot=1
jt=0.0 copyt=1 bandt=1 et=0.000 fexch=F /
```

&partition /

```
&POT kp=1 itt=F ap=8 at=208 rc=1.200 /
&POT kp=1 type=12 shape=10 itt=F p2=1 /
&step /
```

```
&POT kp=1 type=1 itt=F p1=60 p2=1.3 p3=0.65
p4=150 p5=1.3 p6=0.60 /
&POT kp=1 type=12 shape=10 itt=F p2=1 /
&step /
```

```
&POT kp=2 itt=F ap=8 at=208 rc=1.200 /
```



```

&POT kp=2 type=1 itt=F p1=60 p2=1.3 p3=0.65
p4=150 p5=1.3 p6=0.60 /
&POT kp=2 type=12 shape=10 itt=F p2=1 /
&step /

```

```

&pot /

```

```

&overlap /

```

```

&COUPLING icto=1 icfrom=1 kind=1 ip1=8 /
&INEL ib=2 ia=1 k=2 no=2 kp=1 a=12.24 /
&INEL ib=1 ia=2 k=2 no=2 kp=1 a=12.24 /
&INEL ib=1 ia=1 k=2 no=2 kp=1 a=-5.976 /
&INEL ib=2 ia=2 k=2 no=2 kp=1 a=5.477 /
&INEL ib=2 ia=1 k=2 no=3 kp=2 a=2.1433 /
&INEL ib=1 ia=2 k=2 no=3 kp=2 a=2.1433 /
&INEL ib=1 ia=1 k=2 no=3 kp=2 a=-1.0458 /
&INEL ib=2 ia=2 k=2 no=3 kp=2 a=0.9585 /
&INEL/

```

```

&coupling /

```

Output code for fresco input written by xfresco v.1.1.0
at Mon Sep 23 16:16:16 2002

Example 3: $^{16}\text{O} + ^{208}\text{Pb}$ inelastic scattering To illustrate the use of collective form factors in fresco, we have selected the inelastic scattering of $^{16}\text{O} + ^{208}\text{Pb}$ at 80 MeV. In this example, some excited states of the projectile and target are included. In order to account for the excitations of both nuclei, some deformed potentials are defined. The deformation of the ^{16}O is treated within a rotational model whereas those of the ^{208}Pb are treated without assuming any model, by supplying the relevant matrix elements.

After the central Coulomb component of the KP=1 potential, the following deformed potential is included:

```

\&POT kp=1 type=10 itt=F p1=0.000 p2=0.0 p3=37.6~ /

```

- **type=10**: indicates the projectile is being deformed and a rotational model is to be assumed.
- **p3**: corresponds to $M_n(E3) = \langle \chi | M(E_{30}) | \chi \rangle$

Also, the Coulomb potential $kp=1$ is deformed to coupling the target excites in a model independent way:

```
\&POT kp=1 type=13 shape=10 itt=F p1=0.000
p2=54.45 p3=815.0 p4=0.00 p5=0.2380e+5 p6=0.00 p7=0.00 /
```

- **type=13**: indicates that the target nucleus is going to be deformed and that relevant matrix elements are to be supplied explicitly.
- **p1** to **p5**: this is informative only, as the matrix elements will be given explicitly by means of `&step/` namelists, such as:

```
\&step ib=1 ia=3 k=3 str=815.0 /
```

in which the state number $ia = 1$ to coupled to the state $ib = 3$ by means of the octupole Coulomb operator ($k = 3$) and with strength $str = 815$. This corresponds to $(B(E3; 0 \rightarrow 3) = 664225 e^2 fm^6)$.

After these step namelists, the central nuclear potential is defined using `type=1` potentials. As for the Coulomb potential, this is later on deformed using a rotational model:

```
\&POT kp=1 type=10 shape=11 itt=F p3=2.15 /
```

This will couple the states of the projectile using the octupole Coulomb operator and the deformation length $p3=2.15$. This value is consistent with our assumption of a rotational model for ^{16}O and the value of $M_n(E3)$ used for the Coulomb part. As it can be easily checked, the values of β_3 and $M_n(E3)$ are related by the relation (35).

Then, the states or the target are coupled in a model independent way using a `type=13` potential:

```
\&POT kp=1 type=13 shape=10 itt=F p2=54.45 p3=815.0  
p5=0.2380e+5 /
```

- **p2,p3 and p5** are, according to Eq. (34), the deformations lengths $R_0\beta_\lambda$.

The remaining lines define by means of `&step/` namelists, the matrix elements.

```
&STEP ib=1 ia=3 k=3 str=0.8000 /  
&STEP ib=3 ia=1 k=3 str=0.8000 /  
&STEP ib=1 ia=4 k=2 str=0.4000 /  
&STEP ib=4 ia=1 k=2 str=0.4000 /  
&STEP ib=1 ia=5 k=5 str=0.4680 /  
&STEP ib=5 ia=1 k=5 str=0.4680 /  
&step /
```

Example 3: CC with collective form factors

160+208Pb 80 MeV

NAMELIST

```
&FRESCO hcm=0.100 rmatch=17.000 rintp=0.50
hnl=0.033 rnl=3.00 centre=0.00 jtmin=0.0 jtmax=100.0
absend=0.1000 dry=F jump(1:6:1)=0 0 0 0 0 0 jbord(1:6)=
0 0 0 0 0.0 0.0 thmin=80.00 thmax=180.00
thinc=2.50 cutl=0.00 cutr=0.00 cutc=0.00 ips=0.0100
iter=18 iblock=2 pralpha=F pade=1 nnu=24
erange=1.2000 dk=0.0200 chans=1 smats=2 veff=1 kfus=20
pel=1 exl=1 lab=1 lin=1 lex=1 elab=80.0000
nlab(1:3)=0 0 0 fatal=T nosol=F psiren=T
unitmass=1.000000 finec=137.03599 /
```

```
&PARTITION namep='16-0' massp=15.9949 zp=8
namet='PB-208' masst=207.9770 zt=82 qval=0.0000 pwf=T
nex=5 /
```

```
&STATES jp=0.0 bandp=1 ep=0.0000 cpot=1 jt=0.0
bandt=1 et=0.0000 fexch=F /
&STATES jp=3.0 bandp=-1 ep=6.1300 cpot=1 jt=0.0
copyt=1 et=0.0000 fexch=F /
&STATES jp=0.0 copyp=1 ep=0.0000 cpot=1 jt=3.0
bandt=-1 et=2.6100 fexch=F /
&STATES jp=0.0 ep=0.0000 cpot=1 jt=2.0 bandt=1
et=4.0700 fexch=F /
&STATES jp=0.0 ep=0.0000 cpot=1 jt=5.0 bandt=-1
et=3.2000 fexch=F /
```

```
&partition /
```

```
&POT kp=1 itt=F ap=208.000 at=16.000 rc=1.200 /
&POT kp=1 type=10 itt=F p3=37.600 /
&POT kp=1 type=13 shape=10 itt=F p2=54.45 p3=815.0 p5=0.2380e+5 /
&STEP ib=1 ia=3 k=3 str=815.0 /
&STEP ib=3 ia=1 k=3 str=815.0 /
&STEP ib=1 ia=4 k=2 str=54.45 /
&STEP ib=4 ia=1 k=2 str=54.45 /
```

```
&STEP ib=1 ia=5 k=5 str=0.2380E+05 /
&STEP ib=5 ia=1 k=5 str=0.2380E+05 /
&step /

&POT kp=1 type=1 shape=1 itt=F p1=0.000 p2=1.179
p3=0.658 p4=10.000 p5=1.000 p6=0.400 /
&POT kp=1 type=-1 itt=F p1=60.500 p2=1.179
p3=0.658 /
&POT kp=1 type=10 shape=11 itt=F p3=2.150 /
&POT kp=1 type=13 shape=11 itt=F p2=0.400 p3=0.800 p5=0.468 /
&STEP ib=1 ia=3 k=3 str=0.8000 /
&STEP ib=3 ia=1 k=3 str=0.8000 /
&STEP ib=1 ia=4 k=2 str=0.4000 /
&STEP ib=4 ia=1 k=2 str=0.4000 /
&STEP ib=1 ia=5 k=5 str=0.4680 /
&STEP ib=5 ia=1 k=5 str=0.4680 /
&step /

&pot /
&overlap /
&coupling /
```

5 DWBA

Let consider the transfer reaction

$$A + b \rightarrow a + B \quad (A = a + v, B = b + v), \quad (37)$$

When the coupling to intermediate channels is weak, it is reasonable to evaluate the transition amplitude in Born Approximation (BA). In the case of rearrangement reactions there are several ways to describe the interaction between the different fragments, one for each partition. For example, if we choose to describe the scattering in terms of the nuclei of the entrance partition, the projectile target interaction will be written as

$$V_{Ab} = V_{vb} + U_{ab} \quad (38)$$

The interaction V_{vb} is the the potential which binds the v valence particle to the b core. In general, it will be described as a real potential (for which we use the notation V). The potential U_{ab} is the optical potential describing the scattering between b and v . It will typically contain both real and imaginary parts (we use the letter U). In this representation, known as prior form, the transition amplitude for the transfer process is given by

$$\begin{aligned} T_{\text{prior}} &= \langle \chi_{\beta}^{(+)} \phi_a \phi_B | V_{vb} + U_{ab} - U_{\alpha} | \chi_{\alpha}^{(+)} \phi_A \phi_b \rangle \\ &= \int d\mathbf{R}_{\alpha} d\mathbf{R}_{\beta} \chi_{\beta}^{(-)}(\mathbf{R}_{\beta})^* I_{\beta\alpha}(\mathbf{R}_{\beta}, \mathbf{R}_{\alpha}) \chi_{\alpha}^{(+)}(\mathbf{R}_{\alpha}), \end{aligned} \quad (39)$$

with

$$I_{\beta\alpha}(\mathbf{R}_{\beta}, \mathbf{R}_{\alpha}) = (\phi_a \phi_B | V_{vb} + U_{ab} - U_{\alpha} | \phi_A \phi_b) \quad (40)$$

Analogously, for the exit channel: $V_{aB} = V_{av} + U_{ab}$. In this case, the expression (39) reduces to:

$$T_{\text{post}} = \langle \chi_{\beta}^{(+)} \phi_a \phi_B | V_{av} + U_{ab} - U_{\beta} | \chi_{\alpha}^{(+)} \phi_A \phi_b \rangle. \quad (41)$$

where, U_{β} is the optical potential describing the elastic scattering in the exit channel.

In either prior and post form the differential cross section is calculated as:

$$\frac{d\sigma}{d\Omega} = \frac{\mu_{\beta}\mu_{\alpha}}{(2\pi\hbar^2)} \left(\frac{k_{\beta}}{k_{\alpha}} \right) |T(\mathbf{k}_{\beta}, \mathbf{k}_{\alpha})| \quad (42)$$

According to the previous expressions a basic ingredient required to calculate the transfer amplitude in the prior DWBA approximation is the internal wave functions for the initial (ϕ_A, ϕ_b) and final (ϕ_a, ϕ_B) nuclei. In this scheme, the valence particle v is bound to the b core to give the composite B . In the simplest picture, the valence particle can be considered a pure single-particle state. This means that, within this extreme model, there is only one possible configuration of the core and the valence particle to give the nucleus B and thus, the wave function for this nucleus can be written as:

$$\phi_B^{JM}(\xi, \mathbf{r}) = \left[\phi_b^I(\xi) \otimes \varphi_{\ell sj}(\mathbf{r}) \right]_{JM} \quad (43)$$

In a more realistic model, however, the state of the composite contains components of many single-particle states coupled to all possible core states and thus, the wave function $\phi_B^{JM}(\xi, \mathbf{r})$ is built as a superposition of the form:

$$\phi_B^{JM}(\xi, \mathbf{r}) = \frac{1}{\sqrt{n_B}} \sum_{I\ell j} A_{\ell sj}^{IJ} \left[\phi_b^I(\xi) \otimes \varphi_{\ell sj}(\mathbf{r}) \right]_{JM}, \quad (44)$$

where the coefficients $A_{\ell sj}^{IJ}$ are the so called coefficients of fractional parentage (cfp) or spectroscopic amplitudes, and their square moduli $S_{\ell sj}^{IJ} = |A_{\ell sj}^{IJ}|^2$ the spectroscopic factors. The spectroscopic factor $S_{\ell sj}^{IJ}$ can be regarded as the probability of finding the valence particle v in a single particle state ℓ, s, j coupled to the core with spin I . The quantity n_B is the number of nucleons (or clusters!) in the composite system that are identical to that transferred. The factor $1/\sqrt{n_B}$ is introduced just for convenience.

Example: the ground state of the ^{209}Bi nucleus can be modeled to a good approximation as a valence proton coupled to the core ^{208}Pb . Due to the double close shell nature of the core, the valence proton can be regarded as a nearly pure single-particle state, occupying the $1h_{9/2}$ orbital. Then, we have: $I = 0, J = 9/2, (s, \ell, j) = (1/2, 5, 9/2)$ and $S_{\ell sj}^{IJ} \approx 1$. Moreover, as there is only one particle with this configuration, $n_B = 1$ in this case.

Notice that the integral $I_{\beta\alpha}(\mathbf{R}_\beta, \mathbf{R}_\alpha)$ involve the overlap between the composite and core wave functions. Using the expansion (44) the integral on the core internal variables ξ can be explicitly performed giving just unity by normalization.

$$\left(\phi_B^{JM}(\xi, \mathbf{r}), \phi_b^I(\xi) \right) \equiv \int d\xi \phi_B^{JM}(\xi, \mathbf{r}) \phi_b^I(\xi) = \frac{1}{\sqrt{n_B}} \sum_{\ell j} A_{\ell sj}^{IJ} \varphi_{\ell sj}(\mathbf{r}) \quad (45)$$

The bound wave functions $\varphi_{lsj}(\mathbf{r})$ obey the Schrodinger equation³:

$$[T + V_{vb}(\mathbf{r}) + \epsilon - E] \varphi_{lsj}(\mathbf{r}) = 0, \quad (46)$$

where ϵ is the binding energy of the valence particle.

The information required by FRESKO to construct the wave functions is provided in the section of form factors, which corresponds to the namelist `&overlap/` in the fortran 90 version. However, the cfp's and the valence-target and core-target potentials are given in the couplings section, through the `&coupling/` namelist.

It is important to note that the calculation of the transition amplitude involves the integration in the channel coordinates \mathbf{R}_α and \mathbf{R}_β (see Fig. 3), which, after the integration on the angular coordinates, becomes a integral in R_α and R_β . Then, the coupled channels equations becomes:

$$\begin{aligned} [E_\alpha - T_{\alpha L}(R_\alpha) - U_\alpha(R_\alpha)] f_\alpha(R_\alpha) &= \int_0^{R_m} U_{\alpha\beta}(R_\alpha, R_\beta) f_\beta(R_\beta) dR_\beta \\ [E_\beta - T_{\beta L}(R_\beta) - U_\beta(R_\beta)] f_\beta(R_\beta) &= \int_0^{R_m} U_{\beta\alpha}(R_\alpha, R_\beta) f_\alpha(R_\alpha) dR_\alpha, \end{aligned} \quad (47)$$

The integrals

$$S(R_\beta) = \int_0^{R_m} U_{\beta\alpha}(R_\alpha, R_\beta) f_\alpha(R_\alpha) dR_\alpha$$

are evaluated in steps of HCM and up to RMATCH. Previously, Fresco has to evaluate and store the function $U_{\beta\alpha}(R_\alpha, R_\beta)$. It results numerically advantageous to perform the change of variables: $R_\beta \rightarrow D_{\beta\alpha} = R_\beta - R_\alpha$ and thus the functions that are actually stored are $U'_{\beta\alpha}(D_{\beta\alpha}, R_\beta)$. The variable $D_{\beta\alpha}$ is discretized in intervals of HNL, from `CENTRE-RNL/2` to `CENTRE+RNL/2`, i.e., range of RNL centred at CENTRE.

Example 4: DWBA As an example, we will consider the transfer the pickup reaction $^{14}\text{N}(^7\text{Be}, ^8\text{B})^{13}\text{C}$ at 84 MeV, in which a proton is transferred from the ^{14}N target to the ^7Be projectile. For the ^{14}N we adopt the two cluster model: $^{14}\text{N} \rightarrow ^{13}\text{C} + p$, where the valence proton is assumed to occupy the $1p_{1/2}$ orbital, with an spectroscopic amplitude $A = 0.87$. Concerning

³If the core can be excited, it is necessary to solve a coupled set of equations, involving the possible states of the core.

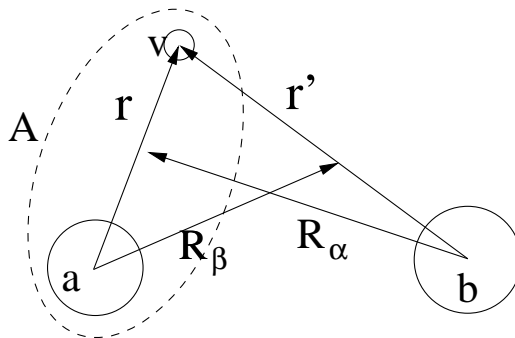


Figure 3: Relevant coordinates for the description of the transfer reaction

the ${}^8\text{B}$ nucleus, we use the model: ${}^8\text{B} \rightarrow {}^7\text{Be} + p$, with the valence proton in a pure single-particle state $1p_{3/2}$ ($A = 1$). According to the mass tables, the binding energies (i.e., one particle separation energies) are $\epsilon = 7.55$ and $\epsilon = 0.137$, respectively.

Notice that two partitions have to be defined, one for the entrance channel (${}^{14}\text{N} + {}^7\text{Be}$) and another for the exit channel (${}^8\text{B} + {}^{13}\text{C}$). To calculate kinetic energies it is also necessary to give the Q -value of the reaction, i.e., the mass difference between the two partitions. This is specified through the variable QVAL (QVAL=-7.41 in this case). For each one of these partitions an optical is defined. These will be used to generate the distorted waves χ_α and χ_β appearing in (39) and (41). In this example, these correspond to potentials KP=1 and KP=2. They are normally chosen to describe the elastic scattering of the corresponding partitions. Thus, potential KP=1 is intended to describe the elastic scattering of the system ${}^{14}\text{N} + {}^7\text{Be}$ at 84 MeV and KP=2 the elastic scattering of ${}^8\text{B} + {}^{13}\text{C}$ at $E \approx 78$ MeV.

In order to calculate the bound wavefunction of the transferred particle in the initial and final nucleus the `&overlap/` namelist are defined. Thus, in the case of the proton bound to the ${}^{13}\text{C}$ core, the following namelist is provided:

```
\&OVERLAP kn1=10 ic1=1 ic2=2 in=2 nn=1 l=1 sn=0.5
j=0.5 kbpot=3 be=7.5506 isc=1/
```

- **kn1**: label to identify this form factor

- **ic1, ic2:** Indexes of the partitions containing the core nucleus (^{13}C) and the composite nucleus (^{14}N). They can be assigned in any order so, for this example, we can define either IC1=1, IC2=2 or IC1=2, IC2=1.
- **in:** bound state of projectile (IN =1) or target (IN=2)
- **nn:** number of nodes. We assume that this the last proton of the ^{14}N occupies a $1p_{1/2}$ single particle states and thus nn=1
- **l:** orbital angular momentum ℓ
- **sn:** spin of transferred particle
- **j:** vector sum $l+sn$
- **kbpot:** is the label of the binding potential. Notice that in this example a potential kp=3 is previously defined in a &pot/ namelist.
- **be:** binding energy (energy separation) of the valence proton.
- **isc:** with the choice isc=1 the TYPE=1 (central) component of the binding potential (KP=3) will be varied to give binding energy BE.

Analogously, an &overlap/ namelist is defined to describe the wave function of the valence proton in the ^8B nucleus.

Next, the kind of transfer is defined through a &coupling/ namelist:

```
\&COUPLING icto=2 icfrom=1 kind=7 ip1=1 ip2=-1 ip3=5 /
```

- **icto, icfrom:** indicates that the valence particle is initially in the ICTFROM partition and is transferred to the ICTO partition. In our example, the valence proton is initially bound to the nucleus ^{14}N , that belongs to the first defined partition; thus, ICTFROM=1.
- **kind:** is the type of coupling. kind=1-4 corresponds to single-particle excitations of projectile/target, whereas kind=5-8 are used to define transfer couplings. For finite-range reactions, we will define a kind=7 coupling.
- **ip1:** to specify prior (ip1=1) or post (ip1=0) interaction.

- **ip2:** is the type of remnant: no remnant (ip2=0), real remnant (ip2=1) or complex (ip2=-1). In this example we choose full complex remnant (ip2=-1) in prior representation (ip1=1).
- **ip3:** is the index of the potential used as core-core interaction (note these two cores are the same in either the post or prior representations).

Thus, with this choice of the input variables the transition amplitude contains the potential: $V_{vb} + U_{ab} - U_{\alpha}$, where V_{vb} is the binding potential of the valence proton in the ${}^7\text{Be}$ nucleus, U_{ab} is the core-core potential ${}^7\text{Be} + {}^{13}\text{C}$ (KP=5) and U_{α} is the optical potential describing the elastic scattering for the ${}^7\text{Be} + {}^{14}\text{N}$ system (KP=1). The remnant potential corresponds to the difference $U_{remnant} = U_{ab} - U_{\alpha}$.

Next, the spectroscopic amplitudes appearing in Eq. (44) are provided by means of `&CFP/` namelists:

```
\&CFP in=2 ib=1 ia=1 kn=10 a=0.87 /
```

```
\&CFP in=1 ib=1 ia=1 kn=1 a=1 /
```

The variable IN is used to distinguish between projectile (IN=1) and target (IN=2). Then, the first namelist defines the composite ${}^{14}\text{N}$ in its ground state (IBb=1) as consisting on a ${}^{13}\text{C}$ core in its ground state (ia=1) coupled to the valence particle and with spectroscopic amplitude $A_{nlj} = 0.87$. The bound wave function will be calculated with the information provided in the coupling KN=10.

In the same way, the second `&cfp/` namelist defines the overlap ${}^8\text{B} \rightarrow {}^7\text{Be} + p$. In this case, the cfp amplitude is chosen as 1, meaning that we assume the valence proton to be on a pure single-particle state.

We finally notice that, apart from the usual information provided in the namelist `&fresco/`, the following variables are defined:

```
\&fresco ... rintp=0.20 hnl=0.100 rnl=12.00 centre=0.25 ... /
```

As explained above these variables are related with the integration of the non-local form factors.

Another important variable in this namelist is ITER. The coupled equations for rearrangement reactions are solved by iterations. The variable ITER refers to the number of iterations used by FRESCO. Thus, ITER=1 corresponds to 1-step Born approximation. Physically, this means that the valence particle is allowed to be transferred from the α partition to the β partition, but the backward coupling $\beta \rightarrow \alpha$ is forbidden. This is in general (but not always!) a good approximation for transfer reaction is a small fraction of the elastic cross section, and so the perturbative calculation in one step is justified.

Example 4: DWBA

DWBA 14N(7Be,8B)13C

NAMELIST

```
&FRESCO hcm=0.100 rmatch=60.000 rintp=0.20
hnl=0.100 rnl=12.00 centre=0.25 rsp=0.0 jtmin=0.0
jtmax=150.0 absend=-0.0010 dry=F
thmin=0.00 thmax=60.00 thinc=0.5
ips=0.0000 iter=1 pralpha=F nnu=24 chans=1 smats=2
xstabl=1 pel=1 exl=1 lab=1 lin=1 lex=1 elab=84.0000
fatal=T nosol=F psiren=F /
```

```
&PARTITION namep='Be7' massp=7.0169 zp=4 namet='14N'
masst=14.0033 zt=7 qval=0.0000 pwf=T nex=1 /
&STATES jp=0.0 bandp=1 ep=0.0000 cpot=1 jt=0.0
bandt=1 et=0.0000 fexch=F /
```

```
&PARTITION namep='B8' massp=8.0246 zp=5 namet='C13'
masst=13.0033 zt=6 qval=-7.414 pwf=T nex=1 /
&STATES jp=1.5 bandp=-1 ep=0.0000 cpot=2 jt=0.5
bandt=-1 et=0.0000 fexch=F /
```

```
&partition /
```

```
&POT kp=1 itt=F ap=7.000 at=14.000 rc=0.697 /
&POT kp=1 type=1 itt=F
p1=79.1 p2=0.763 p3=0.88
p4=36.0 p5=0.837 p6=0.98 /
```

```
&POT kp=2 itt=F ap=1.000 at=0.000 rc=2.939 /
&POT kp=2 type=1 itt=F
p1=85.200 p2=3.300 p3=0.910
p4=39.300 p5=3.760 p6=1.020 /
```

```
&POT kp=3 itt=F ap=0.0 at=13. rc=1.3 /
&POT kp=3 type=1 itt=F p1=54. p2=1.3 p3=0.650 /
&POT kp=4 itt=F ap=1.000 at=0.000 rc=2.391 /
```

```

&POT kp=4 type=1 itt=F
p1=44.675 p2=2.391 p3=0.520 /
&POT kp=4 type=3 itt=F p1=4.898 p2=2.391 p3=0.520 /
&POT kp=5 itt=F ap=7.0 at=13. rc=1. /
&POT kp=5 type=1 itt=F p1=54.3 p2=0.92 p3=0.79
p4=29.9 p5=1.03 p6=0.69 p7=0.000 /
&pot /

&OVERLAP kn1=10 ic1=1 ic2=2 in=2 nn=1 l=1 sn=0.5
j=0.5 kbpot=3 be=7.5506 isc=1 ampl=0.0000 /
&OVERLAP kn1=1 ic1=2 ic2=1 in=1 nn=1 l=1 sn=0.5
j=1.5 kbpot=4 be=0.1370 isc=1 /
&overlap /

&COUPLING icto=2 icfrom=1 kind=7 ip1=1 ip2=-1 ip3=5 /
&CFP in=2 ib=1 ia=1 kn=10 a=0.87 /
&CFP in=1 ib=1 ia=1 kn=1 a=1 /
&cfp /

&coupling /

```

6 Continuum Discretized Coupled Channels (CDCC)

(to be written....)

Appendix

Here I list a few complementary programs that help to handle fresco output files.

- **sumbins.f**:
- **bu-ldist.f**:
- **sumxen.f**: sum various l,j,I components for each energy bin to construct an energy spectrum input: file.xst output: file.xen to be fed in through command line (so far can only deal with equal grid for all components)
- **2coltofr.f**: Converts a two column file (typically containing radius and wavefunction) to (1P,6E12.4) format
- **frto2col.f**: Converts from (1P,6E12.4) format to two column fortran

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