united nations
educational, scientific
and cultural
organization

international atomic
energy agency

the
abdus salam
international centre for theoretical physics

SMR/1325-2

Workshop on

Nuclear Data for Science & Technology: Accelerator Driven Waste Incineration

10 - 21 September 2001

Miramare - Trieste, Italy

EMPIRE II

Statistical Model Code for Nuclear Reaction Calculations

M. Herman
IAEA, Vienna
Austria

EMPIRE-II

statistical model code for nuclear reaction calculations

(version: 2.16 Montenotte)

M.Herman

International Atomic Energy Agency, Vienna, Austria

e-mail: herman@ndsalpha.iaea.org

Target goal: statistical model code with following characteristics:

- universality
- completeness
- easy to use
- expandable (modular)

Features:

- broad range of energies (from above resonance region for neutrons, a up to few hundreds of MeV for Heavy Ions).
- projectile: any nucleon or nucleus (including HI).
- ENDF-VI formatting
- automatic retrieval of experimental data from the EXFOR library .
- interactive plots of experimental and calculated results (excitation functions, ang. distr. and double diff.)
- Graphic User Interface (GUI) written in Tcl/Tk

Outputs:

- total, elastic and reaction cross sections
- cumulative residue production cross sections
- multi-chance fission cross sections
- elastic and inelastic angular distributions
- double differential cross sections for inelastic scattering
- particle and γ-spectra
- cross sections for discrete γ-transitions

- discrete levels' population (isomeric ratios)
- recoil spectra (emission and excitation energy correlations taken into account)

Major nuclear reaction mechanisms:

- optical model (SCAT2),
- coupled channels (ECIS),
- simplified CC for HI fusion (CCFUS),
- TUL Multistep Direct (ORION + TRISTAN),
- NVWY Multistep Compound with γ-emission,
- second-chance preeq. emission,
- exciton model (DEGAS),

- Monte Carlo preequilibrium (DDHMS),
- HRTW for widths' fluctuations,
- Hauser-Feshbach model with full γ-cascade and dynamical deformation effects .

A comprehensive library of input parameters:

- nuclear masses (Nix-Moller),
- ground state deformations (Nix-Moller),
- optical model parameters (RIPL-1),
- discrete levels and decay schemes (ENSDF),
- level densities with dynamical effects
- fission barriers (BARFIT),
- moments of inertia (MOMFIT),
- γ-ray strength functions (RIPL-1).

History

The first version of EMPIRE code has been released in 1980. (Hauser-Feshbach and classical HYBRID model, width fluctuation correction in terms of the HRTW approach)

EMPIRE-MSC FKK Multi-step Compound added

HMS-EMPIRE NVWY Multi-step Compound, combinatorial particle-hole level densities

EMPIRE HI Heavy Ion version

EMPIRE-II totally new release

- all scratch files were eliminated (speed up by a factor of 20),
- all dimensions set up through the FORTRAN parameter statement,
- modular structure (communication through the set of global COMMONS)

Codes incorporated in EMPIRE-II:

ECIS-95	coupled channels by J. Raynal
SCAT2	spherical optical model code by O. Bersillon,
CCFUS	simplified coupled channels calculation of HI fusion cross section by C.H. Dasso and S. Landowne,
ORION+TRISTAN	TUL approach to Multistep Direct by H. Lenske,

DDHMS	Monte Carlo preeq. by M. Chadwick
DEGAS	exciton model by E. Betak and P. Oblozinsky
BARMOM	fission barriers and moments of inertia by A. Sierk.

The package includes also the following stand-alone codes:

EMPEND converts EMPIRE results into ENDF-VI format (written by A. Trkov),

X4TOC4 converts experimental data retrieved from EXFOR into computational format (written by R. Cullen),

FIXUP used to reconstruct MT=4, 103, and 107 (written by R. Cullen),

LEGEND calculate linearly interpolable angular distributions from ENDF data (written by R. Cullen),

LSTTAB tabulates ENDF and EXFOR data in PLOTTAB format (written by A.Trkov),

SIXTAB converts ENDF file MF6 to Law 7 representation (written by A.Trkov),

PLOTC4 plots comparison between EMPIRE results and EXFOR data (written by R. Cullen and extended by A. Trkov),

ZVView plotting package by V. Zerkin.

The models

Fusion/reaction cross section

The reaction cross section is calculated in terms of transmission coefficients $T_l^a(\epsilon)$ using the expression

$$\sigma_a(U,J,\pi) = \frac{\pi}{k^2}\frac{(2J+1)}{(2I+1)(2i+1)} \sum_{S=|I-i|}^{I+i} \sum_{l=|J-S|}^{J+S} f(l,\pi) T_l^a(\epsilon),$$

- k wave number of relative motion,
- i, I, J, and S indicate projectile, target, compound nucleus, and channel spin, respectively,

- l orbital angular momentum of the projectile a.
- $f(l,\pi)$ ensures parity conservation (unity if $p * P * (-1)^l = \pi$ and zero otherwise).
  - Here p, P, and π are projectile, target, and compound nucleus parities
  - ϵ and U stand for the projectile and compound nucleus energy.

A<5 transmission coefficients from optical model routine SCAT2

Heavy Ions:

(i) the simplified coupled channels approach (CCFUS code).

(ii) the distributed fusion-barrier model.

$$f(B') = n_0 \exp\left(\frac{B - B'}{2\sigma_B^2}\right)^2$$

for $|B - B'| < t\sigma_B$ and $f(B') = 0$ otherwise.

$$p(E, l) = \int_{-\infty}^{\infty} f(B') T_l(E - B') dB' .$$

The transmission coefficient in the Hill-Wheeler approach

$$T_l(E - B') = \frac{1}{1 + \exp\left[-2\pi(E - B' - E_{rot})/(\hbar\omega)\right]},$$

E_{rot} rotation energy at angular momentum l.

(iii) the fusion cross sections for each l read from the external file *FUSION*.

(iv) the total fusion cross section specified in input (single incident energy only).

(v) the critical angular momentum l_{cr} for compound nucleus formation specified in input (single incident energy only).

In the latter two cases the transmission coefficients are assumed to be of the form

$$T_l^a(\epsilon) = \frac{1}{1 + exp(-\frac{l_{cr} - l}{\delta l})},$$

where δl is an input parameter.

Coupled Channels and DWBA

- **ECIS** code by J. Raynal
- Important for deformed nuclei
- Provides:
  - total cross section
  - elastic cross section
  - absorption cross section
  - inelastic cross sections to collective levels
  - transmission coefficients

- EMPIRE calls ECIS in a transparent way.
- RIPL or internal omp are used.
- Collective levels taken from RIPL or set up automatically.
- Deformed nuclei treated as rotational, spherical as vibrational.
- Results are transferred to EMPIRE and used in subsequent calculations.

ECIS can be invoked by EMPIRE in 3 ways:

DIRECT=1 CC for collective levels, total, elastic and absorption, SCAT2 transmission coefficients used for PE and HF calculations.

DIRECT=2 as above but CC is used for all transmission coefficients.

DIRECT=3 DWBA for collective levels, total, elastic and absorption, SCAT2 transmission coefficients used for PE and HF calculations.

Multistep Direct

Tamura, Udagawa and Lenske (TUL)

combination of

- direct reaction (DR),
- microscopic nuclear structure and
- statistical methods.

Outline of the theory

$$H = H^{opt} + H^{intr} + V^{res} \quad .$$

- H^{opt} optical model part
- H^{intr} intrinsic Hamiltonian
- V^{res} residual effective projectile-target interaction
- H^{opt} and V^{res} are non-hermitian operators due to the flux absorbed into the closed channels

Lippmann-Schwinger equation for the open channel T-matrix

$$T^{(n)}_{\gamma 0} = < \chi^{(-)}_E | (\gamma | V^{res} (G^{chan}(E) V^{res})^{n-1} | 0) | \chi^{(+)}_0 >$$

describes the $n-$step transition from the entrance channel with incoming scattering wave $\chi^{(+)}_0$ and the ground state configuration $|0) = |aA)$ to an exit channel γ with outgoing wave $\chi^{(-)}_E$ at the energy E

- $G^{chan}(E)$ Green's function for the channel.
- Scattering waves are optical model wave functions.

- Real states γ are expanded into *n*-particle *n*-hole model states *c*. With

$$H^{intr} = H_0^{intr} + V^{intr} \quad .$$

model states c are eigenstates of H_0^{intr}

- Residual interaction V^{intr} couples states from different particle-hole classes only.

- configuration mixing between $np{-}nh$ classes is of stochastic nature

- Level density is

$$\widehat{\rho}(E) = \sum_n \widehat{\rho}_n(E).$$

with

$$\widehat{\rho}_n(E) = \sum_{c=[npnh]} |c) P_c(E) (c|$$

and the probability per energy to find the system in the configuration c is given by the spectroscopic densities,

$$P_c(E) = -\frac{1}{\pi} Im[\int dE' g(E-E')(c|G^{intr}(E')|c)] \,,$$

with $G^{intr}(E)$ being the intrinsic Green's function.

- never-come-back hypotheses

- Cross section is an incoherent super-position of $n-$step contributions

$$\frac{d^2\sigma}{d\Omega dE} = \sum_n \frac{d^2\sigma^{(n)}}{d\Omega dE},$$

where the multistep cross sections are defined as

$$\frac{d^2\sigma^{(n)}}{d\Omega dE} = \sum_{c=[npnh]} P_c(E)|T_{c0}^{(n)}|^2 .$$

Expanding V^{res} into multipoles V_λ the $\sigma^{(1)}$ is determined by an average over transitions into the $1p-1h$ states c around excitation energy E with form factors

$$F_\lambda^{c0} = (c|V_\lambda|0) .$$

- V^{res} is represented in terms of state independent multipole form factors F_λ and nuclear transition operators O_λ

$$V^{res}(r,\xi) = \sum_\lambda F_\lambda(r) O_\lambda(\xi).$$

  - r denotes the relative motion coordinate

  - $\xi = (\xi_a, \xi_A)$ are the intrinsic coordinates

- The multipole form factors F_λ in a self-consistent approach are obtained by averaging V^{res} over O_λ:

$$F_\lambda(r) = (c|O_\lambda^\dagger \hat{\rho}(E) V^{res}|c)/S_\lambda(E,c).$$

For one-step reactions the initial state is the ground state $c = 0$. S_λ is the nuclear response function for the external operator O_λ describing the transition rate per unit energy from the state c into the ensemble of states c' centered at energy E.

- For higher steps the average multipole form factors are used

$$F_\lambda = \frac{tr(\hat{\rho} O_\lambda^\dagger \hat{\rho} V^{res})}{tr(\hat{\rho} O_\lambda^\dagger \hat{\rho} O_\lambda)},$$

- The one-step cross section is expressed as

$$\frac{d^2\sigma^{(1)}}{dEd\Omega} = \sum_\lambda S_\lambda(E) \overline{\frac{d\sigma^{(1)}}{d\Omega}}\,|_\lambda\,,$$

where $\overline{\sigma^{(1)}}$ is a reduced DWBA cross section calculated with the average form factors.

- The state-independent and slowly varying two-step amplitudes read

$$T^{(2)}_{\lambda_1,\lambda_2} = < \chi_E^{(-)} | F_{\lambda_2} G^{opt} F_{\lambda_1} | \chi_\alpha^{(+)} >\,,$$

with G^{opt} being Green's function for the optical model potential.

- The exit channel configurations are $2p-2h$ states which are excited from $1p-1h$ states c_1.

- The final result for the two-step MSD cross section is of very intuitive structure

$$\frac{d^2\sigma^{(2)}}{dEd\Omega} = \sum_{\lambda_1\lambda_2} \int dE_1 S_{\lambda_2}(E, E_1) S_{\lambda_1}(E_1, 0) \overline{\frac{d\sigma^{(2)}}{d\Omega}}(E, E_1) \mid_{\lambda_1\lambda_2}.$$

$\overline{\sigma^{(2)}}$ is an averaged cross section defined in terms of the $T^{(2)}-$matrix elements

Notes on RPA-Description of Transition Strength Functions

- A reliable description of response functions is provided by the Random Phase Approximation theory (RPA).

- The $ph-$classes are built from correlated basis states.

- RPA accounts for collective and non-collective features on the same theoretical footing (weakly excited background states and the strongly excited giant resonances (GR), low-lying surface vibrations).

- Energy weighted sum rules are conserved

- The enhancement of the response due to ground state correlations is included.

- The quasi-particle RPA (QRPA) is used $\Rightarrow$ canonical transformation to quasi-particles (two quasi-particle ($2qp$) rather than $1p-1h$ states).

- $2qp$ energies are taken to be complex by adding a state dependent damping width $\Gamma^{\downarrow}_{\alpha}$.

- Only inelastic events are considered.

- Formally, the response functions are expressed through the RPA polarization propagator $\chi^{RPA}(E)$

$$S_\lambda(E,0) = -\frac{1}{\pi} Im[\chi^{RPA}(E)]\,.$$

- The average response functions are approximated by

$$S_\lambda(E,E_1) \simeq S_\lambda(E-E_1,0)\,,$$

S_λ depends only on energy difference $E-E_1$

- The form factors are found to be given by folding V^{res} with $\overline{\rho_\lambda}$
$\Rightarrow$ consistent description of nuclear structure and reaction dynamics .

- TRISTAN assumes $O_\lambda = \kappa_\lambda U_\lambda$,

  - radial part of U_λ is chosen as the derivative of the ground state potential

  - coupling constants κ_λ are treated as empirical parameters.

- The MSD response functions are calculated with single particle levels from a spherical Nilsson Hamiltonian with standard parameters.
  - The ground state is obtained from a BCS calculation with $\Delta_p = \Delta_n = 12.0/\sqrt{(A)}$ MeV
  - Multipole fields with a radial shape $\sim r^\lambda$ are taken.
  - Coupling constants κ_λ are determined such that excitation energies of low-lying surface oscillations and of the Giant Dipole Resonance are reproduced.
  - The maximum l-transfer λ is between 1 and 4 depending on the maximum l .

Implementation of ORION and TRISTAN codes in EMPIRE

- Input parameters are passed to ORION and TRISTAN directly from the EMPIRE.
- Parameters specific to ORION and TRISTAN are set to default values in EMPIRE (can be modified).
- Default MSD calculation can be performed without any additional input.
- EMPIRE calls ORION with appropriate energy losses (Q-triangle) and form factors (compressional for $\lambda = 0$).
- TRISTAN code modified to authomatize blocking.

- κ_0 selfconsistent coupling
- κ_1 from GDR energy
- κ_2, κ_3, κ_4 from excitation energies of low-lying 2^+, 3^-, and 4^+collective levels.
- charge exchange channels not allowed.

Second-chance PE emission after MSD

A semi-classical approach by M. Chadwick

- Residual after MSD emission contains 1p-1h.
- The excited particle can be neutron or proton.
- It can be emitted with the probability given by the s-wave transmission coefficient.
- Results in a modest increase of the central part of the emission spectra.

Multistep Compound

Nishioka, Verbaarschot, Weidenmueller, Yoshida (NVWY)

- series of transitions along the chain of classes of closed channels of increasing complexity.
- classes defined in terms of the number of excited particle-hole pairs (n) plus the incoming nucleon.

$$N = 2n + 1$$

- two-body force $\Rightarrow$ only neighboring classes are coupled ($\Delta n = \pm 1$).

- Average MSC cross-section

$$\frac{d\sigma_{ab}}{dE} = (1 + \delta_{ab}) \sum_{n,m} T_n^a \Pi_{n,m} T_m^b \,,$$

(kinematical and angular-momentum dependent factors omitted).

- The transmission coefficients T_n^a coupling channel a and class n are given as

$$T_n^a = \frac{4\pi^2 U_n^a}{\left(1 + \pi^2 \sum_m U_m^a\right)^2} \,,$$

where
$U_n^a = \rho_n^b < W_{n,a} >$
ρ_n^b bound level density of class n,
$W_{n,a}$ the average matrix elements connecting channel a with the states in class n.

- The probability transport matrix Π_{mn} is defined via its inverse,

$$(\Pi^{-1})_{nm} = \delta_{nm}(2\pi\rho_n^b)(\Gamma_n^{\downarrow} + \Gamma_n^{ext}) - (1-\delta_{nm})2\pi\rho_n^b\overline{V_{n,m}^2}2\pi\rho_m^b\,.$$

with
$\overline{V_{n,m}^2}$ matrix element coupling states in classes n and m,
$\Gamma_n^{\downarrow}$ average spreading width of states in class n,
Γ_n^{ext} average total decay width in class n.

- The spreading width $\Gamma_n^{\downarrow}$ is again related to the mean squared matrix element $\overline{V_{n,m}^2}$

$$\Gamma_n^{\downarrow} = 2\pi\sum_m \overline{V_{n,m}^2}\rho_m^b\,.$$

- Chaining hypothesis $\Rightarrow$ $\overline{V_{n,m}^2}$ couples only neighboring classes ($\overline{V_{n,m}^2} = 0$ unless $\mid n-m \mid = 1$).

- The decay width Γ_n^{ext} is determined by the sum of the transmission coefficients T_n^a over all open channels

$$\Gamma_n^{ext} = (2\pi\rho_n^b)^{-1}\sum_a T_n^a\,.$$

More explicitly

$$\Gamma_n^{ext} = (2\pi\rho_n^b)^{-1}\sum_\alpha\sum_{m=n-1}^{m=n+1}\int T_{n\to m}^{\alpha}(\varepsilon)\rho_m^b(E-Q_p-\varepsilon)d\varepsilon\,.$$

ε stands for the ejectile p energy,
Q_p for its binding in a composite system, and
α symbolically accounts for the angular momentum coupling

- Chaining hypothesis $\Rightarrow$ only $\mid n-m \mid \leq 1$ emissions are allowed.

- Note that, differently from the FKK formulation, in the NVWY theory transmission coefficients $T_{n\to m}$ carry two class indexes.

- All microscopic quantities $< W_{n,a} >$ and $\overline{V_{n,m}^2}$ are expressed in terms of the macroscopic ones.
  - $< W_{n,a} >$ is equated to optical model transmission coefficient
  - $\overline{V_{n,m}^2}$ is related to the imaginary part of the optical model potential $W(\epsilon)$ with $\Gamma_n^{\downarrow} = 2W(\epsilon)$.
- Matrix Π^{-1} is inverted numerically and used to calculate MSC emission spectra.
- EMPIRE decides whether the MSC calculation should be followed by the Hauser-Feshbach one or not.

Conditional level densities

- The conditional density of states having all p particles bound (i.e. below the binding energy B) reads

$$\rho_{ph}^{B}(E) = \frac{g^{p+h}}{p!h!} \sum_{i=0}^{I} \binom{p}{i} (-1)^i \frac{(E - iB)^{p+h-1}}{(p+h-1)!}$$

for $IB < E \leq (I+1)B$, with $I = 0, 1, ...(p-1)$, and

$$\rho_{ph}^{B}(E) = \frac{g^{p+h}}{p!h!} \sum_{i=0}^{p-1} \sum_{m=0}^{h-1} \binom{p}{i} (-1)^i \frac{[(p-i)B]^{p+m}}{(p+m)!(h-1-m)!} (E - pB)^{h-1-m}$$

for $E > pB$. The superscript B indicates that quantity refers to the bound states embedded in the continuum.

- density of final states accessible to different transition modes compatible with two-body interaction ($\Delta n = -1, 0, +1$).

  - $\Delta = -1$ transition

$$Y_n^{n-1} = \frac{\rho^B_{21}(E-U)\rho^B_{p-2,h-2}(U)}{\rho^B_{ph}(E)}.$$

  - $\Delta = 0$ transition

$$\begin{aligned} Y_n^n &= Bg^2h\frac{\rho^B_{p-1,h}(U)}{\rho^B_{ph}(E)} \\ &+\alpha\frac{1}{2}(h+1)(h+2)\frac{g}{\rho^B_{ph}}\Big[\frac{U-E+2B}{h+2}g\rho^B_{p-2,h+1}(U) \\ &+\beta\rho^B_{p-2,h+2}(E-2B)-\rho^B_{p-2,h+2}(U)\Big], \end{aligned}$$

with $\alpha = 1$for $E \leq 2B + U$, $\beta = 1$ for $E > 2B$, and both equal to 0 elsewhere.

  - $\Delta = +1$ transition

$$Y_n^{n+1} = g\frac{1}{2}h(h+1)\frac{\rho^B_{p.h+1}(U)}{\rho^B_{ph}(E)}$$

- damping width

$$\begin{aligned} Y_n^{n+1}\downarrow &= g\frac{(h+1)(h+2)}{\rho^B_{ph}(E)}\{\frac{1}{2}h\rho^B_{p,h+2}(E)-\alpha\frac{1}{2}h\rho^B_{p,h+2}(E-B) \\ &+(h+3)\frac{1}{2}\rho^B_{p-1,h+3}(E)-\frac{1}{2}\alpha\big[(h+3)\rho^B_{p-1,h+3}(E-B) \\ &+\frac{B^2g^2}{2(h+2)}\rho^B_{p-1,h+1}(E-B)+Bg\rho^B_{p-1,h+2}(E-B)\big]\}, \end{aligned}$$

with α equal 1 for $E > B$ and 0 for $E \leq B$.

γ-emission in Multistep Compound

Hoering and Weidenmueller model.

- Assumptions:
  - γ emission occurs through the deexcitation of the Giant Dipole Resonance (GDR) built within MSC classes.
  - Brink-Axel hypothesis $\Rightarrow$ each nuclear state serves as the basis of a GDR excitation with identical properties.
  - Tamm-Dancoff approximation $\Rightarrow$ GDR is a linear combination of correlated 1p-1h states.

- Each MSC class *M*, splits into four subclasses M_n.
  - $M_{1,2,3}$, contain GDR built on states in class *M-1* with spins *J-1*, *J*, and *J+1*, respectively, and opposite parity.
  - M_4 are pure single particle excitations and contain no GDR.
- The average MSC cross section is given by

$$\overline{\sigma_{a,\gamma}^{MSC}} = T_{a,Mm} \Pi_{Mm,Nn} T_{Nn,\gamma},$$

where

$$(\Pi^{-1})_{Mm,Nn} = 2\pi\rho_{Mm} v_{Mm,Nn} 2\pi\rho_{Nn} + \delta_{M,N}\delta_{m,n} 2\pi\rho_{Mm}(\Gamma^{\uparrow}_{Mm} + \Gamma^{\downarrow}_{Mm})$$

and $T_a = \sum_{Mm} T_{aMm}$ are optical model transmission coefficients.

- Transmission coefficients for the *E1*-γ channel

$$T_\gamma^{E_1} = \frac{1}{2\pi}\sigma_{abs}(E_\gamma^{E_1})\frac{(E_\gamma^{E_1})^2}{(\hbar c)^2}.$$

- The absorption cross section has a Lorentzian form

$$\sigma_{abs}(E_\gamma^{E_1}) = \sigma_{res}\frac{(E_\gamma^{E_1})^2\Gamma_{res}^2}{((E_\gamma^{E_1})^2 - E_{res}^2)^2 + (E_\gamma^{E_1})^2\Gamma_{res}^2}.$$

- $v_{Mm,Nn}$ coupling non-collective states is determined from the imaginary part of the optical model potential.

- Individual $(\Pi^{-1})_{Mm,Nn}$ matrix elements .
  - $(\Pi^{-1})_{Mm,(M+1)n} = 2\pi\rho_{Mm}v^2_{Mm,(M+1)n}2\pi\rho_{(M+1)n}$, there are four different types of matrix elements:
    - the one describing the decay of a GDR,
    - the one responsible for the single particle transitions leaving the GDR unchanged,
    - the one describing transitions among non-collective states,
    - the one describing GDR creation.
  - **(i)** $(\Pi^{-1})_{Mm,(M+1)4}$, $m = 1$, 2 or 3 decay of a GDR via coupling to the next class (spreading width)

$$2\pi\rho_{Mm}v^2_{Mm,(M+1)4}2\pi\rho_{(M+1)4} = 2\pi\rho_{Mm}\Gamma^{\downarrow}_{GDR}.$$

  - **(ii)** $(\Pi^{-1})_{Mm,(M+1)n}$, m, n=1, 2, 3 transition of a GDR-state in class M to

a GDR-state in class $(M+1)$ (GDR is just a "spectator").

$$(\Pi^{-1})_{Mm,(M+1)m} = 2\pi\rho_{Mm}v^2_{n.c.}2\pi\rho^{acc}_{Mm\to(M+1)m},$$

$v_{n.c.}$ is non-collective matrix element.

– **(iii)** $(\Pi^{-1})_{M4,(M+1)4}$
transitions between non-collective states only.

$$(\Pi^{-1})_{M4,(M+1)4} = 2\pi\rho_{M4}(E)v^2_{n.c.}2\pi\rho^{acc}_{M4\to(M+1)4}(E).$$

– **(iv)** $(\Pi^{-1})_{M4,(M+1)m}$ with m = 1,2,3
creation of a GDR in the next exciton class.
It is possible only if a hole has enough energy to create GDR.

$$(\Pi^{-1})_{M4,(M+1)m} = 2\pi\rho_{M4}(E)\Gamma^{\downarrow}_{GDR}\frac{\rho(p,h-1,E-E_{GDR})}{\rho(p,h,E)}.$$

- $(\Pi^{-1})_{(M+1)m,Mn}$ is obtained using the symmetry properties of the matrix Π^{-1}.

- Diagonal elements

$$(\Pi^{-1})_{Mm,Mm} = \sum_{n=1}^{4}(\Pi^{-1})_{Mm,(M+1)n} + \sum_{n=1}^{4}(\Pi^{-1})_{Mm,(M-1)n} + \sum_{c}T_{Mm,c}.$$

$\Pi^{-1}$is inverted numerically and used to calculate γ-emission spectra.

Exciton Model for Preequilibrium Emission

- DEGAS code by E.Betak and P. Oblozinsky
- Semi-classical PE model for nucleon induced reactions
- Strict angular momentum coupling (FKK-like)
- EMPIRE version limited to:
  - single PE emission
  - primary γ-cascade
  - 4 exciton stages

- Absorption cross section renormalized to the EMPIRE one
- Results:
  - neutron, proton and γ spectra
  - spin dependent population of residuals
- Proved to give γ-spectra similar to more microscopic Direct-Semidirect model
- Applicable up to about 30 MeV

Monte Carlo Preequilibrium Emission (DDHMS)

- Formulated by M. Blann and coded by M. Chadwick
- Unlimited multiple precompound emissions
- Residuals' production for nucleon induced reactions
- Double-differential spectra
- Recoil spectra
- Thermodynamically correct binding energies
- Applicable up to about 250 MeV

DDHMS calculation flow:

1. draw collision partner for the incoming nucleon (2p-1h state created)
2. draw energy (ϵ) of the scattered nucleon (if bound go to 5)
3. draw scattering angles for both particles
4. decide whether scattered nucleon will be emitted, re-scattered or trapped
   (a) if emitted appropriate cross section is augmented
   (b) if re-scatters additional particle-hole is created and we return to 2
   (c) if trapped leave it and go to 5
5. draw excitation energy of a particle in the remaining 1p-1h configuration (between $0 \div (U - \varepsilon)$), if unbound go to 3, if bound choose another existing 1p-1h pair and repeat 5.

- All excitons given a chance (including holes)
- Equal *a priori* probabilities
- Cascade ends when all excitons are bound
- Residual's excitation and spin are known and used for feeding H-F decay

Probability distributions

- Collision partners (assuming $\sigma_{np} = 3\sigma_{nn}$) for incident neutron

$$P_{nn} = \frac{(A-Z)}{(A-Z)+3Z}$$

$$P_{np} = 1 - P_{nn}$$

for incident proton

$$P_{pp} = \frac{Z}{Z+3(A-Z)}$$

$$P_{pn} = 1 - P_{pp}$$

- Energy of scattered particles

$$P(\varepsilon)d\varepsilon = \frac{\rho_{n-1}(E-\varepsilon)g}{\rho_n(E)}d\varepsilon$$

with $n = 2\,or\,3$ and

$$\rho_2(E) = \frac{g(gV)}{2} \;\; if \;\; E > V$$

$$\rho_2(E) = \frac{g(gE)}{2} \;\; if \;\; E \leq V$$

$$\rho_3(E) = \frac{g^3\,[V(2E-V)]}{4} \;\; if \;\; E \geq V$$

V being potential well depth

- Emission probability

$$P_\nu = \frac{\lambda_c}{\lambda_c + \lambda_+(\varepsilon)}$$

with emission rate

$$\lambda_c \sim \frac{\sigma_\nu(\varepsilon - Q)(2S+1)\mu_\nu}{g}$$

here: σ_ν - inverse cross section, Q - binding energy, g - single particle density, S - nucleon spin, μ_ν- reduced nucleon mass.

$\lambda_+(\varepsilon)$ from mean free path of a nucleon in nuclear matter (as in the hybrid model)

Compound Nucleus (Hauser-Feshbach)

- Each Compound Nucleus state contributes with a cross section

$$\sigma_b(E,J,\pi) = \sigma_a(E,J,\pi)\frac{\Gamma_b(E,J,\pi)}{\sum_c \Gamma_c(E,J,\pi)}$$

These have to be summed over spin J and parity π, and integrated over excitation energy E (in case of daughter CN)

- Particle decay width

$$\Gamma_c(E,J,\pi) = \frac{1}{2\pi\rho_{CN}(E,J,\pi)} \sum_{J'=0}^{\infty} \sum_{\pi'} \sum_{j=J'-J}^{J+J'} \int_0^{E-B_c} \rho_c(E',J',\pi') T_c^{l,j}(E-B_c-E')dE',$$

B_c - binding energy of particle c in the compound nucleus,
ρ - level density (for discrete levels $\rho = \delta(E-E_i)\delta_{(J',J_i)}\delta_{(\pi',\pi_i)}$)
$T_c^{l,j}(\epsilon)$ - transmission coefficient for particle c having channel energy $\epsilon = E - B_c - E'$ and orbital angular momentum l.

- Fission width

$$\Gamma_f(E,J,\pi) = \frac{1}{2\pi\rho_{CN}(E,J,\pi)} \int_0^{E-E_{sad}(J)} \rho_f(\epsilon,J,\pi) T_f^{HW}(E-E_{sad}(J)-\epsilon)d\epsilon,$$

- $E_{sad}(J)$ is the energy of the saddle point with angular momentum J (sum of the fission barrier $B_f(J)$ and the rotational energy of the nucleus).

$$E_{sad}(J) = B_f(J) + \frac{\hbar^2 J(J+1)}{2(\Im_\perp)_{sad}}.$$

$\Im_\perp$ is a moment of inertia perpendicular to the symmetry axis

- fission transmission coefficient (Hill-Wheeler approximation)

$$T_f^{HW}(E-E_{sad}(J)-\epsilon) = \frac{1}{1+exp[-\frac{2\pi}{\hbar\omega}(E-E_{sad}(J)-\epsilon)]}.$$

Widths' fluctuations (HRTW)

$$S_{ab} = < S >_{ab} + S_{ab}^{fl}$$

cross sections

$$\sigma_{ab}^{CN} = < |S_{ab}^{fl}|^2 >$$

K-matrix representation of of the S-matrix

$$S = (1+iK)(1-iK)^{-1}$$

where

$$K_{ab} = K_{ab}^{(0)} + \sum_\mu \frac{\gamma_{\mu a}\gamma_{\mu b}}{E_\mu - E}$$

real and symmetric K $\Longleftrightarrow$ unitary and symmetric S

Statistical model for S-matrix

- $\gamma_{\mu a}$ and E_μ taken as random variables
  - $\gamma_{\mu a}$ - Gaussian distribution with 0 mean
  - E_μ - Wigner distribution with anticorrelation

Sets of random S-matrices generated numerically

cross sections deduced directly from

$$\sigma_{ab}^{CN} = < |S_{ab}^{fl}|^2 >$$

on the other hand...

in case of no direct reactions

$$< S >_{ab} = \delta_{ab} e^{i\varsigma_{ab}} (1 - T_a)^{1/2}$$

where

$$T_a = 1 - | < S >_{aa} |^2$$

assume CN cross section **factorize(!)**

$$< \sigma_{ab}^{fl} > = \xi_a \xi_b \quad a \neq b \qquad and \qquad < \sigma_a^{fl} > = W_a \xi_a^2$$

setting

$$\xi_a = \frac{V_a}{\sqrt{\sum_c V_c}}$$

we get

$$\sigma_{ab}^{CN} = V_a V_b \left(\sum_c V_c \right)^{-1} \left[1 + \delta_{ab} \left(W_a - 1 \right) \right]$$

unitarity yields

$$V_a = T_a \left[1 + \frac{V_a}{\left(\sum_c V_c \right)} \left(W_a - 1 \right) \right]^{-1}$$

V_a can be found by iteration

numerical experiment:

$$\text{set of random S} \Longrightarrow W_a$$

HRTW:

$$\begin{aligned} W_a &= 1 + 2 \left[1 + T^{0.3 + 1.5 T_a / \left(\sum_c T_c \right)} \right]^{-1} \\ &\quad + 2 \left(\frac{T_a - T_{ave}}{\sum_c T_c} \right)^2 \end{aligned}$$

with $T_{ave} = \frac{1}{N} \sum_{c=1}^{N} T_c$

PROBLEMS:

1. $T_{ave} \to 0$ for many weak γ or fission channels

2. unphysical limit $W_a \to 5$ for a strong channel mixed with very weak ones

SOLUTION:

1. redefine $T_{ave} = \frac{\sum_c T_c^2}{\sum_d T_d}$

2. maximum entropy (Mello-Seligman)

$$W_a = 2 + \frac{2\,(n+1)}{n\,(n+3)} | < S_{aa} > |^2 + \ldots$$

number of channels n can be either:

$$n = \frac{\sum_c T_c}{T_a}$$

or

$$n = \frac{\sum_c T_c}{T_{ave}}$$

suggested form

$$W_a = 1 + 2\left[1 + T_a^{4(n+1)/n(n+3)}\right]^{-1} + corr$$

the only fit:

$$W_a = 1 + 2\left[1 + T_a^F\right]^{-1} + 87\left(\frac{T_a - T_{ave}}{\sum_c T_c}\right)^2 \left(\frac{T_a}{\sum_c T_c}\right)^5$$

with

$$F = 4\frac{T_{ave}}{\sum_c T_c}\left(1 + \frac{T_a}{\sum_c T_c}\right)\left(1 + 3\frac{T_{ave}}{\sum_c T_c}\right)^{-1}$$

giving $\chi^2 = 1.01$ per degree of freedom

- allows to treat radiation channels
- fulfills the Agasi-Weidenmueller limit

$$Wa \to 2 \quad if \quad \sum_c T_c \gg 1 \quad and\ all \quad T_c \ll 1$$

- corresponds exactly to Mello-Seligman expression in the strong absorption limit

Observed a few cases with

$Wa > 3 \Longrightarrow$ FACTORIZATION BREAKDOWN

HRTW (implementation)

HRTW is applied to each J^π state in the highest energy bin in the first CN

- fusion cross section to J^π has to be decomposed into its l components
- first sweep: T_l for all channels are stored and elastic channels are recorded
- second sweep: V_l and HF-type denominator are calculated, elastic channels enhanced
- third sweep: partial widths are normalized

Level densities

- Equal parity distribution $\rho(E,J,\pi) = \frac{1}{2}\rho(E,J)$ is assumed.

Gilbert-Cameron type level densities

- Constant temperature formula (up to U_x)

$$\rho_T(E) = \frac{1}{T} exp\left[(E - \Delta - E_0)/T\right],$$

T is the nuclear temperature,
E is the excitation energy ($E = U + \Delta$ with Δ being the pairing correction),
E_0 is an adjustable energy shift.

- Fermi gas formula (above U_x)

$$\rho_F(U) = \frac{exp(2\sqrt{aU})}{12\sqrt{2}\sigma(U)a^{1/4}U^{5/4}}.$$

- Spin cut-off factor $\sigma^2(U) = 0.146A^{2/3}\sqrt{aU}$.

- T, U_x, and E_0, are determined by the requirement that the level density and its derivative are continues at the matching point U_x, The first of the conditions implies

$$\frac{1}{T} = \sqrt{a/U_x} - \frac{3}{2U_x}.$$

- FITLEV option in EMPIRE $\Rightarrow$ cumulative plots of discrete levels on the screen.

- a parameter
  - constant
  - Ignatyuk type

$$a(U) = \tilde{a}[1 + f(U)\frac{\delta W}{U}],$$

- δW is the shell correction,
  $\tilde{a}$ is the asymptotic value of the a-parameter
  $f(U) = 1 - exp(-\gamma U)$.
  - three systematics available in EMPIRE:
    * Ignatyuk et al.
    * Arthur
    * Iljinov et al.
- No collective effects in Gilbert-Cameron approach!

Dynamical approach to level densities

(specific to EMPIRE)

- Features:
  - Collective enhancements due to nuclear vibration and rotation.
  - Super-fluid model below critical excitation energy
  - Fermi gas model above critical excitation energy
  - Rotation induced deformation (spin dependent)

- Prolate nuclei

$$\rho(E,J,\pi) = \frac{1}{16\sqrt{6\pi}}\left(\frac{\hbar^2}{\Im_{\parallel}}\right)^{\frac{1}{2}} a^{1/4} \sum_{K=-J}^{J}\left(U-\frac{\hbar^2K^2}{2\Im_{eff}}\right)^{-\frac{5}{4}} \exp\left\{2\left[a\left(U-\frac{\hbar^2K^2}{2\Im_{eff}}\right)\right]^{\frac{1}{2}}\right\}.$$

- Oblate nuclei

$$\rho(E,J,\pi) = \frac{1}{16\sqrt{6\pi}}\left(\frac{\hbar^2}{\Im_{\parallel}}\right)^{\frac{1}{2}} a^{1/4} \sum_{K=-J}^{J}\left(U-\frac{\hbar^2\left[J\left(J+1\right)-K^2\right]}{2|\Im_{eff}|}\right)^{-\frac{5}{4}} \exp\left\{2\left[a\left(U-\frac{\hbar^2\left[J\left(J+1\right)-K^2\right]}{2|\Im_{eff}|}\right)\right]^{\frac{1}{2}}\right\}.$$

K is spin projection,
$\Im_{eff}$ effective moment of inertia
defined in terms of
perpendicular $\Im_{\parallel}$and parallel $\Im_{\perp}$moments

$$\frac{1}{\Im_{eff}} = \frac{1}{\Im_{\parallel}} - \frac{1}{\Im_{\perp}}.$$

- Rotational enhancement automatically taken into account.

- Vibrational enhancement

$$K_{vib} = exp\left\{1.7\left(\frac{3m_0A}{4\pi h^2 S_{drop}}\right)^{2/3} T^{4/3}\right\}$$

with $S_{drop} = 17/4\pi r_{2_0}$ and $r_0 = 1.26$.

- Rotational and vibrational enhancements are damped with increasing energy

Super-fluid (BCS) model

- With the pairing gap $\Delta = 12/\sqrt{A}$ the critical temperature T_{crt} is

$$T_{crt} = 0.567\Delta.$$

The critical value *a* found by iteration

$$a_{crt}^{(0)} = \tilde{a}\,(1 + \gamma\delta_W)$$

$$U^{(n)} = a_{crt}^{(n)} T_{crt}^2$$

$$a_{crt}^{(n+1)} = \tilde{a}\left[1 + \frac{\delta_W}{U^{(n)}}\left(1 - \exp\left(-\gamma U^{(n)}\right)\right)\right]$$

$\tilde{a}$ asymptotic value of the level density parameter.

- condensation energy E_{cond}

$$E_{cond} = 1.5 a_{crt}\Delta^2/\pi^2,$$

critical energy U_{crt}

$$U_{crt} = a_{crt}T_{crt}^2 + E_{cond},$$

- critical value of the determinant Det_{crt}

$$Det_{crt} = \left(\frac{12}{\sqrt{\pi}}\right)^2 a_{crt}^3 T_{crt}^5,$$

- critical entropy S_{crt}

$$S_{crt} = 2a_{crt}T_{crt}.$$

- Below U_{crt} we define the parameter φ

$$\varphi = \sqrt{1 - U/U_{crt}},$$

then

$$T = 2T_{crt}\varphi \ln^{-1}\left(\frac{\varphi + 1}{1 - \varphi}\right),$$

$$S = S_{crt}T_{crt}(1 - \varphi^2)/T,$$

$$Det = Det_{crt}(1 - \varphi^2)(1 + \varphi^2)^2.$$

- Parallel and orthogonal moments of inertia below the critical temperature T_{crt}

$$\Im_{\parallel}^{BCS} = \Im_{\parallel} T_{crt}(1-\varphi^2)/T$$

and

$$\Im_{\perp}^{BCS} = \frac{1}{3}\Im_{\perp} + \frac{2}{3}\Im_{\perp} T_{crt}(1-\varphi^2)/T$$

- Squares of the effective spin cut-off parameters

$$\sigma_{eff}^2 = \Im_{\parallel}^{BCS} T \qquad for\ \alpha_2 < 0.005\,,$$
$$\sigma_{eff}^2 = \left(\Im_{\parallel}^{BCS}\right)^{1/3} \left(\Im_{\perp}^{BCS}\right)^{2/3} T \qquad for\ \alpha_2 > 0.005\,,$$

with α_2 ground state deformation.

- BCS level densities are

$$\rho_{BCS}(U,J) = \frac{2J+1}{2\sqrt{2\pi}\sigma_{eff}^3\sqrt{Det}} \exp\left(\frac{S-J(J+1)}{2\sigma_{eff}^2}\right)$$

- Corrected for rotational and vibrational collective effects in the non-adiabatic mode

$$\rho(U,J) = \rho_{BCS}(U,J) Q_{rot}^{BCS} K_{rot} Q_{vib} K_{vib}\,.$$

- Rotational enhancement

$$K_{rot} = \Im_{\perp} T$$

damped with

$$Q_{rot}^{BCS} = 1 - Q_{rot}\left(1 - \frac{1}{\Im_{\perp} T}\right)\,,$$

3 variants of dynamical level densities:

(i) EMPIRE-specific:

- a energy dependent following Ignatyuk et al.
- a deformation dependent (surface term)
- experimental values extracted fitting D_{obs}
- EMPIRE-specific systematics built in
- 'local systematics' created during calculations
- BCS below U_{crt}

- adjustment to the discrete levels

(ii) fit to the shell-model s.p.s.:

- energy dependent $a(U) = a_1 + a_2 e^{-a_3 U}$ fitted for about 4000 nuclei
- no adjustment to experimental data

(iii) a = A/constant:

- a is constant
- no adjustment to experimental data

Nuclear deformation and moments of inertia

Nucleus' shape affects:

- parameters of the Giant Dipole Resonance,
- level density parameter a,
- rotational enhancement of the level densities.

Dynamic deformation α_{2dyn} is calculated following Vigdor and Karwowski

$$\alpha_{2dyn} \approx b(-1.25y/(1-x)),$$

b is an adjustable parameter. The angular momentum parameter y

$$y = 1.9249\frac{I(I+1)}{\eta A^{7/3}}$$

fissility parameter

$$x = 0.01965\frac{Z^2}{\eta A}.$$

η is the neutron-proton difference term

$$\eta = 1 - 1.7826(N-Z)^2A^{-2}.$$

Accordingly, the deformation is parametrized as

$$\alpha_2(T,I) = \alpha_{g.s.}h(T) + \alpha_{2dyn}$$

where $h(T) = 1/\{1 + \exp[(T-2)/0.5]\}$ damps the ground state deformation

Moments of inertia for the yrast states

$$\Im_{\|} = \Im_0(1 - \alpha_2 + 0.429\alpha_2^2 + 0.268\alpha_2^3 - 0.212\alpha_2^4 \\ -1.143\alpha_2\alpha_4 + 0.494\alpha_2^2\alpha_4 + 0.266\alpha_4^2)$$

$$\Im_{\perp} = \Im_0(1 + 0.5\alpha_2 + 1.286\alpha_2^2 + 0.581\alpha_2^3 - 0.451\alpha_2^4 \\ +0.571\alpha_2\alpha_4 + 1.897\alpha_2^2\alpha_4 + 0.700\alpha_4^2)$$

with the rigid-sphere moment of inertia

$$\Im_0/\hbar^2 = 0.01448A^{5/3}\ MeV^{-1},$$

and

$$\alpha_4 = \frac{\alpha_2^2(0.057 + 0.17x + c_2y) + c_3\alpha_2y}{1 - 0.37x - c_1y}.$$

Saddle-point moments of inertia provided by the MOMFIT routine (A. Sierk).

Fission barriers

The liquid-drop spin dependent fission barriers, for 19<Z<102, calculated using BARFIT subroutine

For nuclei with Z≥102 the recent parameterization of the Thomas-Fermi fission barriers at zero spin is used .

The full fission barrier

$$B_f(T, J) = B_{ld}(J) - f(T)\, g(J)\, \delta_W.$$

Temperature fade-out

$$f(T) = 1 \qquad for\ T < 1.65MeV$$
$$f(T) = e^{1.066(1.65-T)} \qquad for\ T \geq 1.65MeV.$$

Angular momentum fade-out

$$g(J) = \frac{1}{1 + \exp\left[(J - J_{1/2})/\Delta J\right]} + d\cdot\exp\left[(J - J_G)^2/\Delta J_G^2\right],$$

Dissipation effects

(i) the stationary limit of Kramers

(ii) the exponential factor applied to the Kramers' fission width to account for the transient time after which the statistical regime is reached.

γ-ray emission

E1, E2, and M1 transitions are taken into account.

Transmission coefficient

$$T_{Xl}^{GMR} = 2\pi f_{Xl}(E_\gamma) E_\gamma^{2l+1} .$$

Brink-Axel hypothesis with Giant Dipole Resonance (GDR) shape described by the sum of two generalized Lorenzians (Uhl-Kopecky).

The E1 γ-ray strength function

$$f_{E1}(E_\gamma) = \sum_{i=1}^{2} \sigma_i \Gamma_i \left[\frac{E_\gamma \Gamma_i(E_\gamma)}{(E_\gamma^2 - E_i^2)^2 + E_\gamma^2 \Gamma_i(E_\gamma)^2} + \frac{0.7 \Gamma_i 4\pi^2 T^2}{E^5} \right]$$

energy and temperature (T) dependent width

$$\Gamma_i(E_\gamma, T) = \Gamma_i \frac{E_\gamma^2 - 4\pi T^2}{E_i^2} .$$

GDR parameters estimated from the spin dependent systematics.

Coupling between MSC and MSD chains

Higher MSC classes populated directly from the MSD chain

Incoming flux splits between the first MSD and MSC classes in proportion to the respective state densities and to the average value of the squared matrix elements

$< V_{uu}^2 >$ unbound to unbound

$< V_{ub}^2 >$ unbound to bound .

$$T_1 = T_{om} \frac{< V_{ub}^2 > \rho_1^b(E)}{< V_{ub}^2 > \rho_1^b(E) + < V_{uu}^2 > \rho_1^u(E)}$$
$$= T_{om} \frac{R}{(R-1) + \frac{\rho_1(E)}{\rho_1^b(E)}}$$

where $R = < V_{ub}^2 > | < V_{uu}^2 >$
and

$$T_n = T_{om} - \sum_{i=1}^{n-1} T_i \frac{R}{(R-1) + \frac{\rho_n(E)}{\rho_n^b(E)}}$$

Absorption cross section available to MSC (σ_{abs}) reduced by the total MSD emission

$$\sigma_{abs}(J) = \sigma_{OM}(J) \left(1 - \frac{\sigma_{MSD}}{\sigma_{OM}}\right)$$

Model compatibility

Various PE models $\Rightarrow$ double counting

EMPIRE avoids problem assigning following priorities:

ECIS — inelastic scattering to collective levels irrespective of other models.

MSD — inelastic to continuum independently of other settings. Inelastic to discrete levels suppressed if ECIS active.

MSC — inelastic to continuum and charge-exchange to continuum if not suppressed by DEGAS or HMS.

DEGAS — inelastic and charge-exchange to continuum and discrete levels if MSD and MSC are not active. Otherwise only charge-exchange contribution is used. γ emission used if not provided by MSC.

HMS — inelastic and charge-exchange to continuum and discrete levels if MSD and MSC are not active. Otherwise only charge-exchange contribution is used. Suppresses DEGAS results for particle emission. Does not provide γ emission, thus DEGAS or MSC results are used.

The code

Directory structure

- **empire**
  - **source** - source of the EMPIRE code divided into modules and Makefile
  - **data** - library of input parameters (files: *ldp.dat, nix-moller-audi.dat, nparac.dat, orsi.liv*, mass-hms.dat, omp.ripl ripl-omp.index)
  - **work** - input and output files, scripts
  - **EXFOR** - EXFOR library, index file (REAC_SIG.TXT) and retrieval tools
    - **subent** - 183 subdirectories with EXFOR subentries

- **util** - utility codes
  - **empend** - code converting EMPIRE results into the ENDF format
  - **legend** - calculates linearly interpolable angular distributions from ENDF data
  - **lsttab** - tabulates ENDF and EXFOR data in PLOTTAB format
  - **sixtab** - converts ENDF file MF6 to Law 7 representation
  - **fixup** - used to reconstruct MT= 1, 4, 103, and 107

- **util** - utilty codes (cont.)
  - **x4toc4** - code converting retrieved EXFOR data into the computational format
  - **c4sort** - sorts data in the computational format (file .c4)
  - **plotc4** - code plotting the comparison between calculated and experimental data
  - **c4zvd** - ZVView plotting package
  - **auxiliary** - icons , sound and pictures
- **doc** - documentation

Installation

gunzip empire-2.xx.tgz

tar xvf empire-2.xx.tar
cd empire
Install

Install script will execute *make* command wherever needed. By default, *g77* compiler is used.

For full functionality EMPIRE needs:

- FORTRAN 77(90) compiler
- C-compiler (if not integrated with FORTRAN)
- gnuplot
- ghostview
- awk
- bash shell
- Tcl/Tk

Array dimensions

All the dimensions are set in the *dimension.h* file and can be changed if necessary.

NDNUC	maximum number of nuclei involved in the calculation
NDEJC	number of ejectiles (must be 3 or 4)
NDEX	maximum number of energy bins in the continuum discretization
NDLW	maximum number of partial waves to be considered in calculations

NDTL	maximum number of partial waves in SCAT2, can be less than NDLW and must not be larger than 100
NDMSCS	number of steps in Multistep Compound
NDLV	maximum number of discrete levels in any nucleus
NDBR	maximum number of branching ratios for each level

Parameter libraries

- **Masses**
  (*empire-2.xx/data/nix-moller-audi.dat*)
  Calculations of Moller and Nix and recent recommended masses by Audi and Wapstra

- **Discrete levels**
  (*empire-2.xx/data/orsi.liv*)
  This file contains 82030 discrete levels for 2320 isotopes up to A=262 and Z=107. The data were extracted from the ENSDF library in April 1996.

- **Level density parameters**
  (*empire-2.xx/data/ldp.dat*)
  Number of levels which are assumed to constitute a complete set
  1286 nuclides taken form the RIPL-1 library

Parameter libraries (cont.)

- **Level density parameters from the shell-model**
  (*empire-2.xx/data/nparac.dat*)
  This file contains level density parameters for 3962 nuclei in the range between ^{12}C and ^{252}Sg derived from the spacings of the shell-model single-particle spectrum.

- **Index of RIPL-1 optical model parameters**
  (*empire-2.xx/data/*RIPL-1-omp.index)
  The list of keywords and validity ranges for omp's contained in RIPL-1.

- **RIPL-1 optical model parameters**
  ***(empire-2.xx/data/*omp.ripl)**
  Optical model parameters taken from RIPL-1.

Flow of the calculations

1. read EMPIRE input file (*.inp*)

2. construct table of nuclei involved

3. read from the input parameter library (or input/output files if such exist)

   (a) discrete levels,

   (b) binding energies,

   (c) level density parameters,

   (d) shell corrections,

   (e) ground state deformations ,

4. calculate

(a) transmission coefficients ,

(b) level densities,

(c) fission barriers

5. retrieves experimental data from the EXFOR library.

6. writes input/output files

(a) .exf

(b) .omp

(c) .lev

7. ECIS (CC elastic and inelastic scattering)

8. determine fusion cross section

9. select the compound nucleus for consideration

10. MSD (for the first CN only)

11. MSC (for the first CN only)

12. DEGAS (exciton model, for the first CN only)

13. HMS (for the first CN only)

14. HRTW (for the highest energy bin in the first CN only)

15. calculate particle and fission widths with Hauser-Feshbach

16. normalize emission and fission widths with the Hauser-Feshbach denominator and fusion cross section

17. print results for the decay of the considered nucleus

18. select new nucleus and repeat steps 15 through 18 until all requested nuclei are treated.

19. print inclusive spectra, read new incident energy from the input file (*.inp*) and repeat steps 4 and 7 through 19.

Executing EMPIRE

Three modes:

- manual,
- script mode
- Graphic User Interface (GUI)

Script mode

- Scripts use UNIX bash-shell (!)
- Each script is invoked with a name of the input file without(!) *.inp* extension.
  `runE Mo100`

The following scripts are provided:

runE runs EMPIRE, retrieves EXFOR data and translates them into computational format

format run EMPEND to transform *.out* output into ENDF format (produces *.endf* file)

plot runs PLOTC4 to create comparison plots of experimental and calculated cross sections

run does all above (runE + format + plot)

clean removes files with extensions: *.lev, .endf, .lst, .out, .x42c4_errs, .x42c4_lst*, and *.exf*

zvd create ZVView plot for the selected MT excitation function ('ZVV' button in GUI).

zvpl create ZVView plot for the excitation function for any cross section printed in the main output ('Create ZVV' button in GUI).

zvcomb merge several existing ZVView plots into one plot ('Merge ZVV' button in GUI).

Additional scripts facilitate handling of outputs:

store moves *all output* files for all projects (*.inp* files are copied rather than moved) to a subdirectory specified as a parameter to *store*.

run-piece-wise runs up to 3 input files for the same case but in different, non-overlapping energy ranges. Used to apply different model parameters in separate energy ranges.

cleanall removes all output files preserving inputs.

GUI mode

- Invoked by typing: `lrun.tcl`
- Creates input file.
- Runs the code.
- Formats the results and plots comparisons.
- Offers access to most of the scripts with a simple mouse click.

List of files

.inp ♣	EMPIRE input
.fus ♣	fusion cross sections (optional)
-ecis.in	input file for ECIS (last energy)
.lst	EMPIRE output (long)
.out	EMPIRE output (short)
-ecis.out	ECIS output (last energy)
.lev	discrete levels for all nuclei involved in the run

-lev.col	collective levels to be used by ECIS
-omp.int	optical model parameters for various nucleus-ejectile combinations
-omp.ripl	optical model parameters from RIPL
-omp.dir	optical model parameters for direct (ECIS) calculations
.endf	results in the ENDF format
-s.endf	.endf processed with FIXUP, LEGEND and SIXTAB
.exf	relevant experimental data retrieved from EXFOR (if EXFOR installed)

.c4	relevant EXFOR data translated into computational format
.ps	PostScript plots comparing calculations against experimental data (PLOTC4)
-MT.zvd	input file for ZVView
.x42c4_lst	output of X4TOC4 code
.x42c4_errs	list of EXFOR entries not translated by the X4TOC4 code

Creation of the ENDF file

- select ENDF =1 or 2 in the input file (*.inp*)
- ENDF=1 (exclusive spectra)
  - EMPIRE rearranges exclusive emission spectra (d and dd) to conform to the ENDF rules.
  - dd spectra for recoils (for binary reactions exact, for two particle emission channels approximated, no recoils for 3 particle emission).
  - Only neutron induced reactions and outgoing channels up to (n,3npα) can be processed (use up to 20 MeV!).

Creation of the ENDF file (cont.)

- ENDF=2 (inclusive spectra)
  - Inclusive light particle emission spectra (d and dd) in CM .
  - Recoil spectra include correlations among subsequent emissions (LAB).
  - Arbitrary reaction can be handled (high incident energies).

Creation of the ENDF file (cont.)

- EMPIRE output (*.out*) is processed and converted into ENDF format by running EMPEND code (not completed for ENDF=2).
- MF=1, 3, 4 and 6 are created
- MT=5 representation for ENDF=2.
- dd cross sections and angular distributions are expanded in Legendre polynomials.
- Cross sections can be interpolated with a cubic spline.

Input/Output files

.inp (main input)

- EMPIRE reads as much data as possible form the input parameter library (*empire/data*).

- User has to supply only those input parameters that the code **can not** know (incident energy, the projectile, the target and the number of neutron, proton, α, and light-ion emissions)

- Prioritized access to input data

  1. case specific files (*.lev*, *.fus*, *.omp*)

  2. input file (*.inp*)

  3. general input parameter library

Note, that *all (*except *.inp)* files are created by the code in the first run. User **only** has to create an *.inp* file.

Editing *.lev*, *-omp.**, and *.c4* files is a convenient method of adjusting some of the input data without necessity of typing the whole set from scratch.

Input file *.inp* of EMPIRE consists of the mandatory and the optional part.

Mandatory input

```
14.8 ;INCIDENT ENERGY (IN LAB)
56.  26.  ;TARGET A , Z
1.  0.  ;PROJECTILE A, Z
3 ;NUMBER OF NEUTRONS TO BE EMITTED
1 ;NUMBER OF PROTONS TO BE EMITTED
1 ;NUMBER OF ALPHAS TO BE EMITTED
0.  0.  0.  ;NUMBER OF L.I. TO BE EMITTED
```

All reactions up to (n,3npα) will be calculated.

$\sigma_{(n,3np\alpha)} = \sigma_{(n,2npn\alpha)} + \sigma_{(n,np2n\alpha)} + \sigma_{(n,p3n\alpha)} + \sigma_{(n,\alpha 3np)} + \cdots$

light ion d, t, ^{3}He, ^{6}Li, ^{7}Li, and ^{7}Be ejectiles (NDEJC = 4 in the file *dimension.h*)

.lst (long output)

size depends on the controls IOUT and NOUT specified in input (*.inp*)

- code banner
- optional input
- 1-st incident energy
  - Compound Nucleus
    - model parameters
    - ORION results
    - TRISTAN results
    - fusion cross section
    - MSC results (including pure MSC spectra)
    - discrete level population before their γ-de-excitation

  - * intensities of discrete γ-lines
  - * residue production cross section
  - * fission cross section
  - * γ, n, p, α, and light ion spectra
- — 1-st residue
  - * model parameters
  - * discrete level population before their γ-deexcitation
  - * intensities of discrete γ-lines
  - * residue production cross section
  - * second-chance fission cross section
  - * γ, n, p, α, and light ion spectra
- — 2-nd residue
  - * ...
- — last residue
  - * ...

  - — inclusive γ, n, p, α, and light ion spectra

- 2-nd incident energy
  - — ...

- last incident energy
  - — ...
  - — inclusive γ, n, p, α, and light ion spectra

-ecis.in

- ECIS input produced by EMPIRE (for checking) in each run.

-lev.col

- File with collective levels for ECIS produced by EMPIRE in the first run.

-ecis.out

- ECIS output file (for the last energy)

.out (short output)

```
REACTION   6-C - 12 +  13-Al- 27 INCIDENT ENERGY   50.1     MeV
COMPOUND NUCLEUS ENERGY   51.295 MeV
FUSION CROSS SECTION =   1285.1     mb
19-K - 39 production cross section 0.566424E-08 mb
   fission  cross section  0.0000     mb
g  emission cross section 0.15879     mb
n  emission cross section  250.52     mb
p  emission cross section  247.58     mb
He emission cross section  786.84     mb


REACTION   6-C - 12 +  13-Al- 27 INCIDENT ENERGY   100.      MeV
COMPOUND NUCLEUS ENERGY   85.841 MeV
FUSION CROSS SECTION =   1653.8     mb
19-K - 39 production cross section 0.558363E-11 mb
```

With ENDF option this file is read by the EMPEND code.

.fus

- User supplied fusion cross sections.
- If present, will override any disposition in input.
- A simple column of fusion cross sections for subsequent partial waves starting with $I = 0$.
- Code will consider only those below actual value of NDLW.
- Can be used for a single energy only.

.lev

- Discrete levels for all nuclei involved in a calculation.
- Produced by EMPIRE during the first run.

```
 6                    26 12  0___ ENSDF ___
1   0.000  0.0        26 12  1
1   1.809  2.0        26 12  2 100
1   2.938  2.0        26 12  3 110 290
1   3.589  0.0        26 12  4 200
1   3.941  3.0        26 12  5 1 0 238 362


1   4.318  4.0        26 12  6 1 3 297
```

- **.lev** often needs modifications:
  - cut-off some levels
  - missing branching ratios,
  - uncertain spins and/or parities,
  - add levels.

-omp.int

- Optical model parameters for various nucleus-ejectile combinations.
- Produced, from built-in systematics, during the first run.

```
 38-K  +  1-n       19038 +     1

Emin, Emax    0.0000   15.0000    1.0000    0.0000    1.2500

real vol     54.1900   -0.3300    0.0000    0.0000    1.1980    0.6630

imag vol      0.0000    0.0000    0.0000    0.0000    1.2950    0.5900

imag surf     4.2800    0.4000    0.0000    0.0000    1.2950    0.5900

real SO       6.2000    0.0000    0.0000    0.0000    1.0100    0.7500
```

$$V(E) = c_0 + c_1 E + c_2 E^2 + c_3 \ln(E)$$

-omp.ripl

- Optical model parameters for various nucleus-ejectile combinations for which RIPL omp were specified in input.
- Produced, from RIPL-1 omp library, during the first run.
- Reproduces RIPL-1 format.

-omp.dir

- Optical model parameters to be used in ECIS for CC or DWBA calculations
- Produced, from the RIPL-1 omp library or internal systematics during the first run
- Reproduces RIPL-1 or internal format

.endf

- EMPIRE results in the ENDF format resulting from the processing with the EMPEND code.

-s.endf

- **.endf** file processed with FIXUP, LEGEND and SIXTAB.

.exf

- Relevant experimental data retrieved from the EXFOR library (in EXFOR format).

.c4

- EXFOR data translated into the computational format by the X4TOC4 code.
  reaction ^{124}Sn (n,2n)

```
 1 24052   3  16    1.2722+7  8000.000  0.038800  1.5000-3
 1 24052   3  16    1.2744+7  8000.000  0.041200  1.6000-3
 1 24052   3  16    1.3251+7  10000.00  0.121900  5.0000-3
 1 24052   3  16    1.3271+7  10000.00  0.123700  5.1000-3
 1 24052   3  16    1.3888+7  9000.000  0.240600  9.7000-3
 1 24052   3  16    1.3902+7  9000.000  0.250600  0.010100
 1 24052   3  16    1.4251+7  8000.000  0.322000  0.012500
```

.ps

- PostScript plots comparing calculations against experimental data produced by the PLOTC4 code.
- Note that to be plotted the results must be ENDF formatted.

-MT.zvd

- Input file for plotting MT reaction with ZVView (e.g., mn55-102.zvd).
- Created by invoking ZVView from the GUI.
- Different zvd files can be combined into a single plot using the 'Merge ZVV' button of GUI.

empend.log

- produced by the EMPEND code to monitor translation of the EMPIRE output into the ENDF format.

.x42c4_lst

- Log on the translation from EXFOR to computational format.

.x42c4_errs

- List of EXFOR entries not translated by the X4TOC4.

Hints for using EMPIRE

- Run *clean* script when necessary.
- Calculations with the FITLEV option activated should be performed at the highest incident energy expected.
- If ENDF option is selected the incident energies should be in increasing order.
- Check output files *.x42c4_errs* and *empend.log* for possible error messages.
- MSD=2 option must be used with care (existing output of ORION (*TAPE15*) may not be compatible with the current case).

Plans for further development

- dispersive omp (under completion)
- improvement of the fission channel (under way),
- extension of the EMPEND code to projectiles different from neutrons and to energies above 20 MeV (under way)
- preequilibrium emission of clusters in MSC,
- manual (GUI assisted) fitting of omp

Plans for further development (cont.)

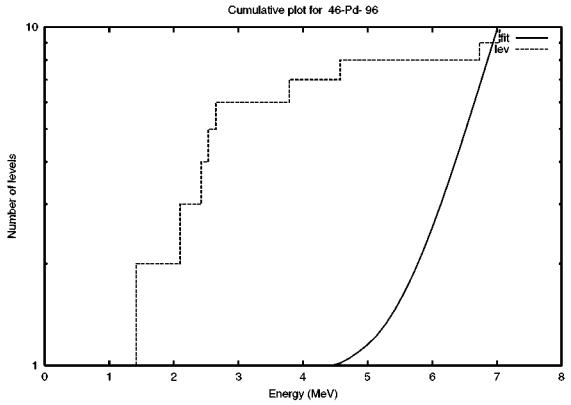
- more extensive use of the RIPL (RIPL-2) library
  - new discrete levels
  - extended omp
  - tables of microscopic level densities
- microscopic p-h level densities for MSC (routine exists),
- automatic adjustment of the γ-ray strength functions to the observed Γ_γ

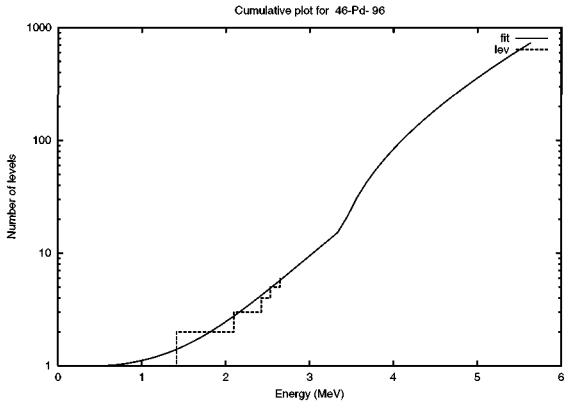
Test cases

Fitting discrete levels

- Running EMPIRE with the FITLEV option is **strongly recommended** !
  Checks discrete level schemes for completeness and consistency with the level density parameterization.
- Cumulative plots displayed on the screen
- One should edit *.lev* file and remove the levels which are in excess.
- The number of levels at the beginning of the appropriate section of the *.lev* file should be modified accordingly

Examples of bad and good fit of discrete levels





Neutron capture

```
 1.9                ;INCIDENT ENERGY (IN LAB)

100.  42.             ;TARGET  A , Z

1.     0.             ;PROJECTILE A, Z

0                   ;NUMBER OF NEUTRONS TO BE EMITTED

0                   ;NUMBER OF PROTONS  TO BE EMITTED

0                   ;NUMBER OF ALPHAS   TO BE EMITTED

0  0.  0.             ;NUMBER OF L.I. TO BE EMITTED

GO

-1.
```

Heavy ion induced reaction

^{48}Ca + ^{248}Cm reaction ⇒ Z=116.

```
240.0                ;INCIDENT ENERGY (IN LAB)
248.  96.            ;TARGET  A , Z
48.   20.            ;PROJECTILE A, Z
6                    ;NUMBER OF NEUTRONS TO BE EMITTED
0                    ;NUMBER OF PROTONS TO BE EMITTED
0                    ;NUMBER OF ALPHAS TO BE EMITTED
0  0.  0.             ;NUMBER OF LI TO BE EMITTED
IOUT       3.
NEX      100.
BETAV      8.6
SHRJ      20.
SHRD       3.
LTURBO     2.
GO
-1.
```

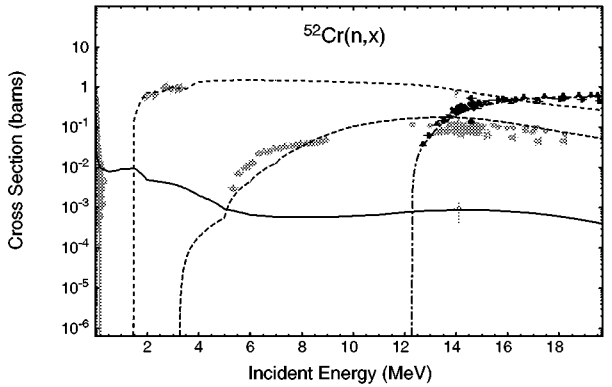

MSD+MSC+HF calculation

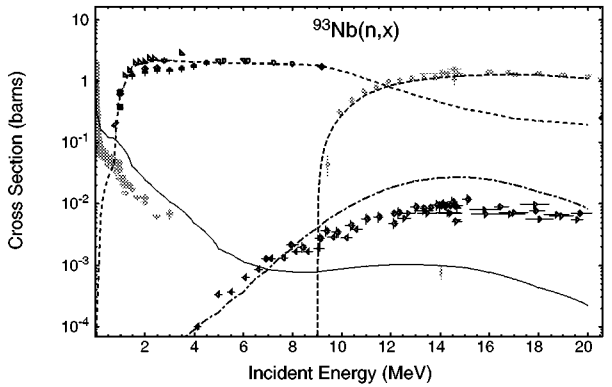
All reactions of the type
^{100}Mo(n, xn yp $z\alpha$)
with x=0, 1, 2, y= 0, 1 and z=0, 1

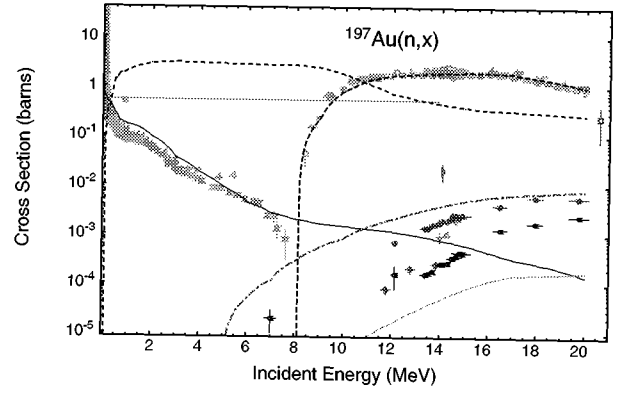
```
  0.1                ;INCIDENT ENERGY (IN LAB)
100.  42.            ;TARGET A , Z
  1.   0.            ;PROJECTILE A, Z
2                    ;NUMBER OF NEUTRONS TO BE EMITTED
1                    ;NUMBER OF PROTONS TO BE EMITTED
1                    ;NUMBER OF ALPHAS TO BE EMITTED
0  0.  0.             ;NUMBER OF L.I. TO BE EMITTED
IOUT       3.
LEVDEN     0.
NEX      100.
MSD        1.
MSC        1.
ENDF       1.
```

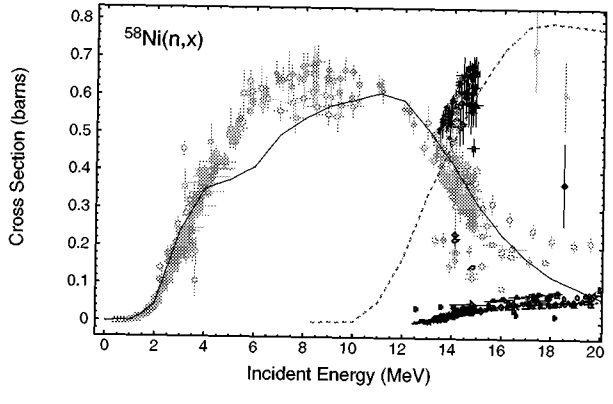
```
OMPOT      6.        1
GO
0.5
1.
2.
3.
...
17.
18.
20.

-1.
```

Examples of default calculations









Adjusted results