The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

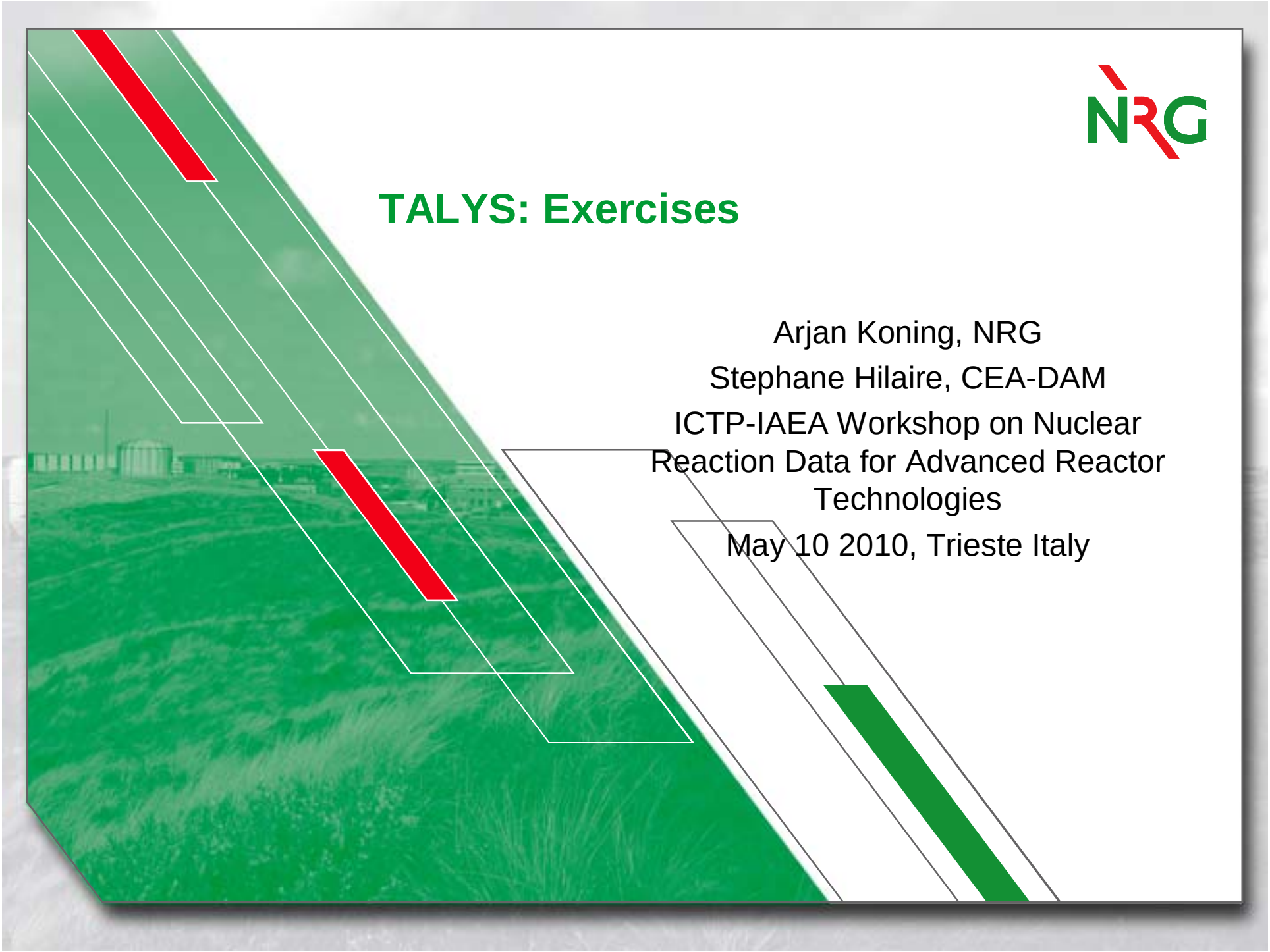
2141

Joint ICTP-IAEA Workshop on Nuclear Reaction Data for Advanced Reactor Technologies

3 - 14 May 2010

TALYS: Exercises

KONIG A.
NRG
Petten
Netherlands



TALYS: Exercises

Arjan Koning, NRG
Stephane Hilaire, CEA-DAM

ICTP-IAEA Workshop on Nuclear Reaction Data for Advanced Reactor Technologies

May 10 2010, Trieste Italy

Installing TALYS

Talys can be downloaded from www.talys.eu

- Linux: tar zxvf talys.tar
- *README*: contents of the package.
- *talys.setup*: script for installation.
- *source/*: source code
- *structure/*: nuclear structure database
- *doc/*: the documentation (manual)
- *samples/*: input and output files of the sample cases.

TALYS setup

- Works under Windows XP
- Works under Linux
- Works with a variety of Fortran-77,90,95 compilers
- Only 2 little system dependencies: subroutine machine.f
- edit **talys.setup**: set compiler name and place of executable
- **talys.setup**
- **rehash**

Alternative (manual) setup

- cd talys/source
- edit machine.f
- replace the pathname by the total pathname of the structure database on your system
- save machine.f
- g77 –c *.f
- g77 *.o –o talys
- mv talys ~/bin or wherever you want to have the executable

Running the TALYS sample cases

- Goto the *samples/* directory
- **verify**
- Wait for 1 hour until all 18 sample cases are finished.....
- ..... or try your own input files.

All 18 sample cases are described in the manual, with input files, output files, plots etc.

See talys/doc/talys1.2.pdf

TALYS sample cases (see manual)

1 All results for 14 MeV n + 93Nb

2 Excitation functions: 208Pb(n,n'), (n,2n), (n,p) etc.

3 Comparison of compound nucleus WFC models: 10 keV n + 93Nb

4 Recoils: 20 MeV n + 28Si

5 Fission cross sections: n + **232Th**

6 Continuum spectra at 63 MeV for Bi(n,xp)...Bi(n,x)

TALYS sample cases (see manual)

7 Pre-equilibrium angular dist. and multiple pre-equilibrium emission

8 Residual production cross sections: p + nat Fe up to 100 MeV

9 Spherical optical model and DWBA: n + 208Pb

10 Coupled-channels rotational model: n + 28Si

11 Coupled-channels vibrational model: n + 74Ge

12 Inelastic spectra at 20 MeV: Direct + Preeq + GR + Compound

TALYS sample cases (see manual)

13 Gamma-ray intensities: 208Pb(n,n'γ) and 208Pb(n,2nγ)

14 Fission yields for 238U

15 Photonuclear reactions: γ + 90Zr

16 Different optical models : n + 120Sn

17 Different level density models : n + 99Tc

18 Astrophysical reaction rates : n + 187Os

Sample 1A: simplest case (1 energy)

Cd talys/samples/1/a/new

The first sample problem concerns the simplest possible TALYS calculation. Consider the following input file that produces the results for a 14 MeV neutron on ^{93}Nb:

```
#
# General
#
projectile n
element nb
mass 93
energy 14.
```

where the purpose of the lines starting with a "#" is purely cosmetical. This input file called *input* can simply be run as follows:

talys < input > output

All important results are in the output file

Sample 1: output

```
############ REACTION SUMMARY FOR E= 14.000 ############

Center-of-mass energy:  13.849

1. Total (binary) cross sections

Total            = 3.98195E+03
Shape elastic    = 2.21132E+03
Reaction         = 1.77063E+03
  Compound elastic= 6.00478E-04
  Non-elastic     = 1.77063E+03
    Direct           = 3.13938E+01
    Pre-equilibrium = 4.15372E+02
    Giant resonance = 6.25327E+01
    Compound non-el = 1.26133E+03
  Total elastic    = 2.21132E+03
```

Sample 1: output (continued)

4. Residual production cross sections

a. Per isotope

Z	A	nuclide	total cross section	level	isomeric cross section	isomeric ratio	lifetime
41	94	(94Nb)	1.18322E+00	0	5.99984E-01	0.50708	
				1	5.83234E-01	0.49292	3.76000E+02 sec.
41	93	(93Nb)	3.23646E+02	0	2.77623E+02	0.85780	
				1	4.60226E+01	0.14220	5.09000E+08 sec.
40	93	(93Zr)	2.98798E+01	0	2.98798E+01	1.00000	
41	92	(92Nb)	1.37164E+03	0	8.51757E+02	0.62098	
				1	5.19887E+02	0.37902	8.77000E+05 sec.
40	92	(92Zr)	1.57424E+01	0	1.57424E+01	1.00000	
40	91	(91Zr)	1.81576E-01	0	1.81576E-01	1.00000	
39	90	(90Y)	2.53059E+01	0	1.28873E+01	0.50926	

Sample 8: residual production with protons

Cd talys/samples/8/new; talys <input > output

(pre-calculated results in talys/samples/8/org)

7.3.8 Sample 8: Residual production cross sections: p + ^{nat}Fe up to 100 MeV

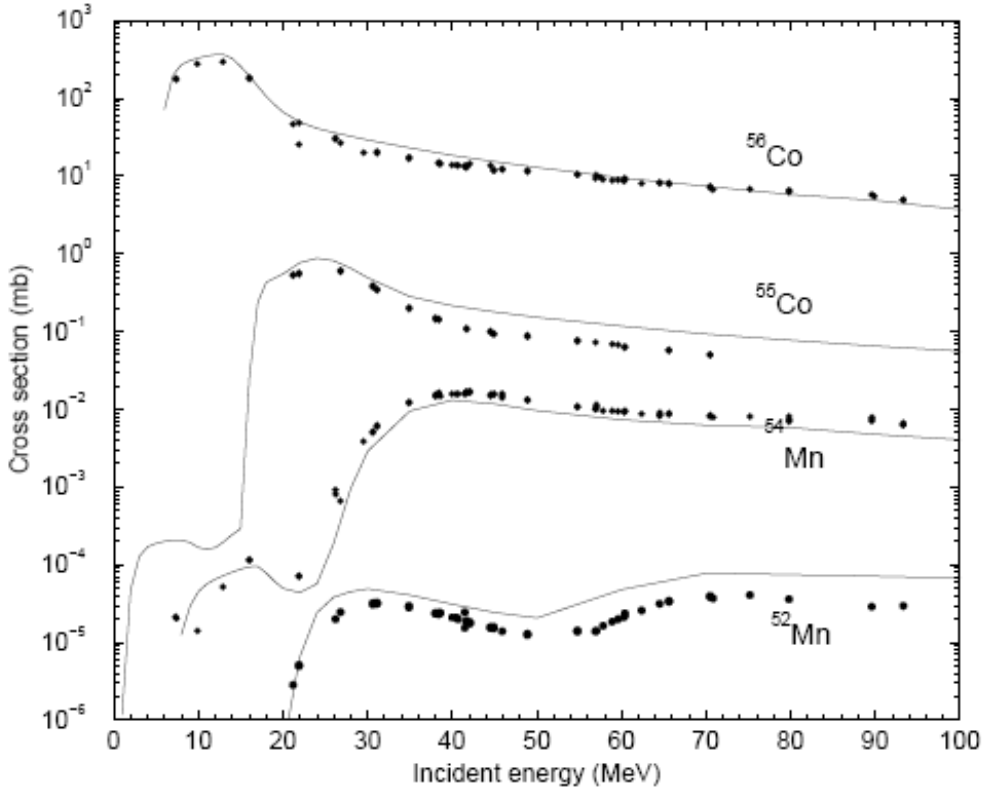
In this sample case, we calculate the residual production cross sections for protons on ^{nat}Fe for incident energies up to 100 MeV. A calculation for a natural target is launched, meaning that successive TALYS calculations for each isotope are performed, after which the results are weighted with the natural abundance. We restrict ourselves to a calculation with all nuclear model parameters set to their default values. The following input file is used:

```
#
# General
#
projectile p
element fe
mass 0
energy energies
#
# Output
#
fileresidual        y
```

Residual production c.s. for Fe

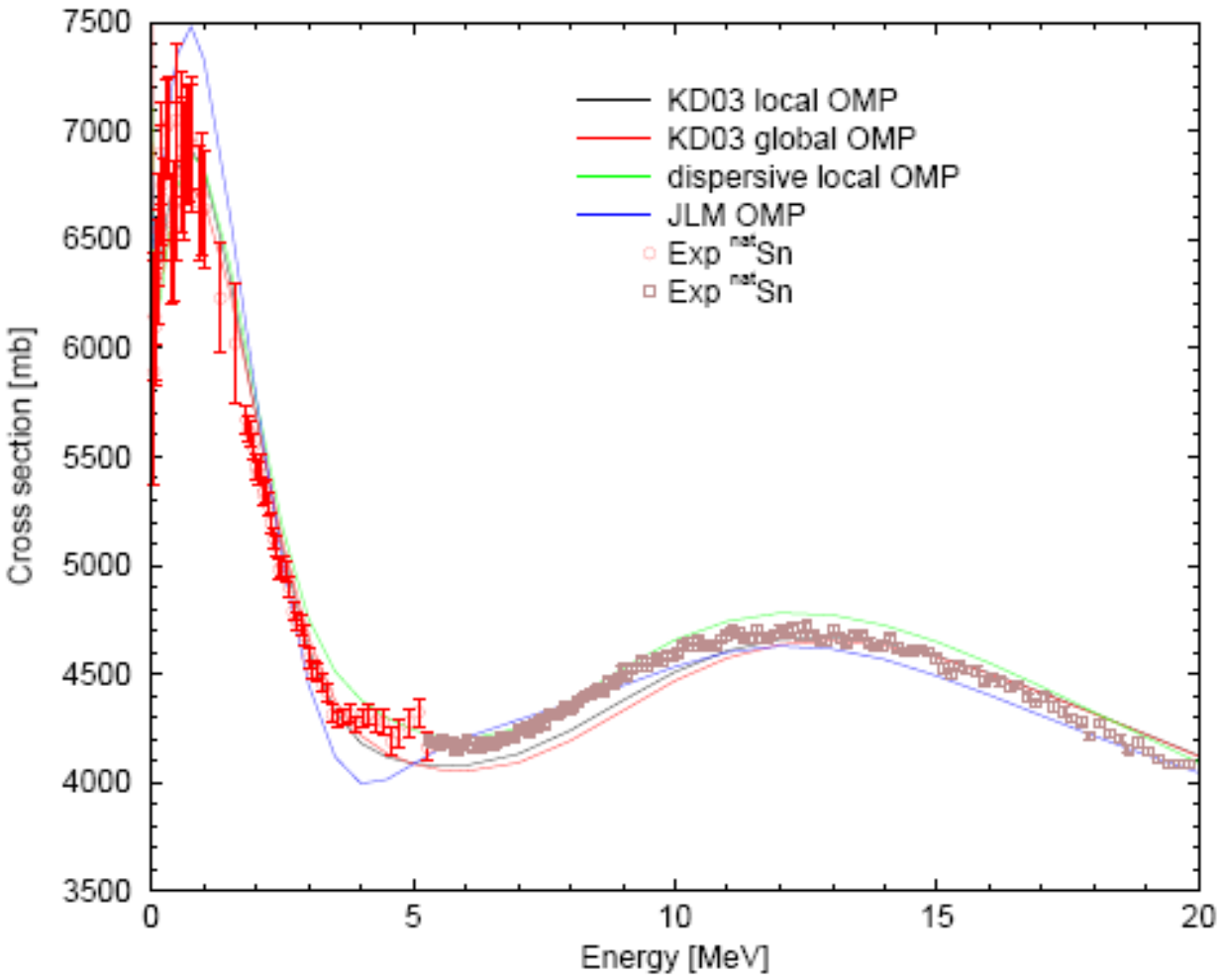
Plot: xmgrace rp027056.tot

results from the files *rp027056.tot*, *rp027055.tot*, *rp025054.tot* and *rp025052.tot* are presented, together with experimental data, in Fig. 7.10.



Sample 16: optical model for 120Sn

- Study impact of changing parameters
- talys < input >output (about 20-30 seconds)
- cp totalxs.tot totalxs.org
- Edit the input file and add the following line:
  - rvadjust n 1.05
  - This means: increase the radius of the real volume potential by 5%
- xmgrace totalxs.tot totalxs.org (to see the difference)
- TALYS has 250 parameters like this (RT*M)


^{120}Sn(n,tot)
KD03 local OMP
KD03 global OMP
dispersive local OMP
JLM OMP
Exp ^{nat}Sn
Exp ^{nat}Sn
Cross section [mb]
Energy [MeV]
7500
7000
6500
6000
5500
5000
4500
4000
3500
0
5
10
15
20