

Report of the Subgroup A 2003-04 Activities

Aix-en-Provence, France - May 26-28, 2004

1. Progress Report on Individual Codes
Coh, Empire, Mcgnash, Talys
2. Development of the **MODLIB** library:
Goal, Status, and Future

Notes on the Subgroup A Meeting on May 25, 2004

Three main groups collaborating (Europe & USA):

- **Talys (NRG & CEA)**
- **Empire (BNL + IAEA collaboration)**
- **McGnash + CoH (LANL)**

*In addition to developing new validated and standardized reaction modeling codes, Subgroup A provides **a useful framework for collaborative work and exchanges** between these 3 projects.*

Progress Report on Individual Codes - I

COH

T.Kawano (LANL) / C, Perl / Under development

Characteristics: coupled-channels calculations available for the entrance channel
RIPL2COH interface

EMPIRE

M.Herman et al. (BNL) / F77 / Stable (2.18)

(R.Capote, P.Oblozinsky, M.Sin, A.Trkov, A.Ventura, V.Zerkin)

Characteristics:

Major nuclear reaction mechanisms included

Comprehensive library of input parameters based on RIPL-2

Powerful graphical interface and plotting capabilities against exp. data

Under development: exclusive spectra, sophisticated fission channel,
photo-nuclear reactions, exciton model for cluster emission, ...

Progress Report on Individual Codes - II

MCGNASH

P.Talou, M.B.Chadwick (LANL) / F95, Perl / Under development

Characteristics:

GNASH “heir”; most important features from GNASH already in place.
Use of the DDHMS code for preequilibrium phase.
Inclusive and Exclusive spectra. Width fluctuation corrections.
Under development: new fission model using Moller’s calculations of fission paths. Test of exclusive spectra calculations. Manual writing.

TALYS

*A.Koning (Petten), S.Hilaire (CEA), and M.C.Duijvestijn (Petten) / F77 /
To be released at ND2004, Oct. 2004.*

Characteristics:

Very complete. Latest nuclear models for direct, compound, pre-equilibrium and fission reactions.
Calculation of most physical quantities of interest.
Automatic link to RIPL database. Automatic ENDF-6 formatting.
Exclusive spectra, prediction of fission fragment distribution with the Brosa model, merging of ENDF evaluated files with TALYS results, etc.
Under development: (“Chadwick”) model for recoils, transfer to F90, final manual, and official publication of the code.

ModLib

A library of Fortran 95 modules for nuclear reaction codes

Goal: constitute a library of well-tested and well-documented modules to be used in existing and future nuclear reaction codes.

Advantages:

Avoid duplication of work

Simplify **inter-comparison of codes**

(act as a reference on which everyone can agree upon)

Get the **BEST CODING AND PHYSICS EXPERTISE** into a public library

Coding in modern Fortran 95- very good for building libraries!

Can already be used in existing F77/C codes (e.g., EMPIRE and TALYS)

What has been done:

Organization

- Structure, hierarchy of the library
- Coding rules and Header template
- Submission rules, standards (Makefile, archive, sample case, ...)
- Web site, mailing lists, ...

Physics

Basic: **Accuracy** (e.g., real kind), **Constants** (fundamental constants)

Physics:

Level Density Representation (Gilbert-Cameron),
Gamma-ray Strength Function (Giant Dipole Resonance),
Width Fluctuation Correction Factors (HRTW, Moldauer, GOE),
Pre-equilibrium DDHMS model (Chadwick-Blann)

ENDF:

CHECKR, FIZCON, STANEF, INTER, PSYCHE (Dunford)

In the Working...

Organization

- Modules testing,
- How to best use the library,
- New web site and FTP server,
- ...

Physics

Existing Modules:

Extend the existing modules to include State-of-the-Art physics models.

New Modules:

To be discussed at the May 25th meeting.

Timeline

Milestone:

MODLIB V.1.0

by the end of '04

- Library file: `libmodlib.a`, so that `> f90 -lmodlib ...`
- Contains 7 modules (+ ENDF processing codes)
- / Accuracy / Constants / Level_Density / Definitions / Width_Fluctuations / G-rays Str. Fct. / (STANEF, CHECKR, ...) / Numerical_Tools (GSL) / RIPL-3?
- Testing in “Mother Codes”

Longer Term:

NEW MODULES

1-2 years

- * Pre-equilibrium code DDHMS [MCGNASH]
- * Kalbach cluster emission [TALYS]
- * Specific level densities [EMPIRE]

& Testing, benchmarking of modules