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Activity Report of the ENEA Nuclear Data Project in 2005

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March 2006

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Activity Report of the ENEA Nuclear Data Project in 2005

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Abstract

Descriptions are given of the nuclear data activities at the Bologna Research Centre of the Italian National Agency for New Technologies, Energy and the Environment (ENEA), in the year 2005. This work has been done within the P9H6 project of the Division for Advanced Physics Technologies.

March 2006

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CPT-symmetric Quantum Mechanics

Non-Hermitian quantum mechanics has played a key role in nuclear physics since the introduction of the optical model in reaction theory. It is of basic interest to investigate the properties of non-Hermitian Hamiltonians, **H**, possessing definite properties under parity transformation, **P**, time reversal, **T**, and charge conjugation, **C**.

The study of Hamiltonians that are invariant under **PT**, but not under **P** and **T** separately, gave rise in 1998 to **PT**-symmetric quantum mechanics. **PT**-symmetric Hamiltonians can have real discrete spectra, in spite of the fact that they contain complex potentials.

Our work has focused on one-dimensional non-relativistic quantum mechanics, and we have searched for the simplest possible form of a “charge-conjugation” operator, **C**, and given explicit examples of Hamiltonians invariant under **CPT** transformations, but not under any of the three separate transformations, or under the product of two of them. **CPT** invariance of the Hamiltonian is equivalent to the intertwining relationship

$$\mathbf{CPH^{+} = HCP}\ , \qquad (1)$$

where $\mathbf{H^{+}}$ is the Hermitian conjugate of **H** and it is assumed that $\mathbf{CP = (CP)^{+}}$**.** **C** is chosen of the form

$$\mathbf{C = d/dx + w(x)}\ , \qquad (2)$$

where **w** is a complex function of the real coordinate x. Relationship (1) connects the real and the imaginary part of the potential, **V(x),** in the Hamiltonian, $\mathbf{H = -d^2/dx^2 + V(x)}$**,** with the real and the imaginary part of **w(x)**. Moreover, **C** and its complex conjugate $\mathbf{C^{*}}$ turn out to be the building blocks of a supersymmetric formulation, which has been worked out in detail for a family of anharmonic-oscillator potentials [A.1].

Nuclear Structure Theory

Level Densities of Transitional Sm Isotopes

A microcanonical formalism suited to the calculation of nuclear level densities at low excitation energy has been developed and applied to the transitional isotopes $\mathbf{^{148,149,150,152}Sm}$ [A.2].

Non-collective level densities are computed in a Monte Carlo approach, where excited proton and neutron configurations, based on single-particle level schemes generated by a spherical Woods-Saxon potential, plus residual p-p and n-n pairing interactions in Bardeen-Cooper-Schrieffer approximation, are sampled at random by means of a Metropolis algorithm.

Collective level densities are computed by means of a version of the interacting boson model (IBM) including not only *s* and *d* bosons, with $L^{\pi} = 0^{+}$ and 2^{+}, respectively, which generate collective levels of positive parity, but also *f* bosons, with $L^{\pi} = 3^{-}$, whose interactions with *s* and *d* bosons produce levels of negative parity. The parameters of the IBM Hamiltonian are adjusted on the experimental discrete spectra of both parities.

Level densities of given angular momentum and parity, as well as total level densities, to be compared with experimental data, are computed by folding non-collective and collective level densities generated by Monte Carlo and IBM, respectively.

The transitional nature of the samarium isotope chain considered in this work (ranging from the spherical nucleus **^{148}Sm** to the deformed nucleus **^{152}Sm**) shows up in the steady increase of collective level densities, in particular those of negative parity, with increasing mass number.

Total level densities of the four isotopes under consideration are plotted in Fig. 1 as a function of excitation energy, E, up to E = 9 MeV , and compared with recent experimental data of **^{148}Sm** and **^{149}Sm** (S. Siem *et al.*, Phys. Rev. C **65** (2002) 044318).

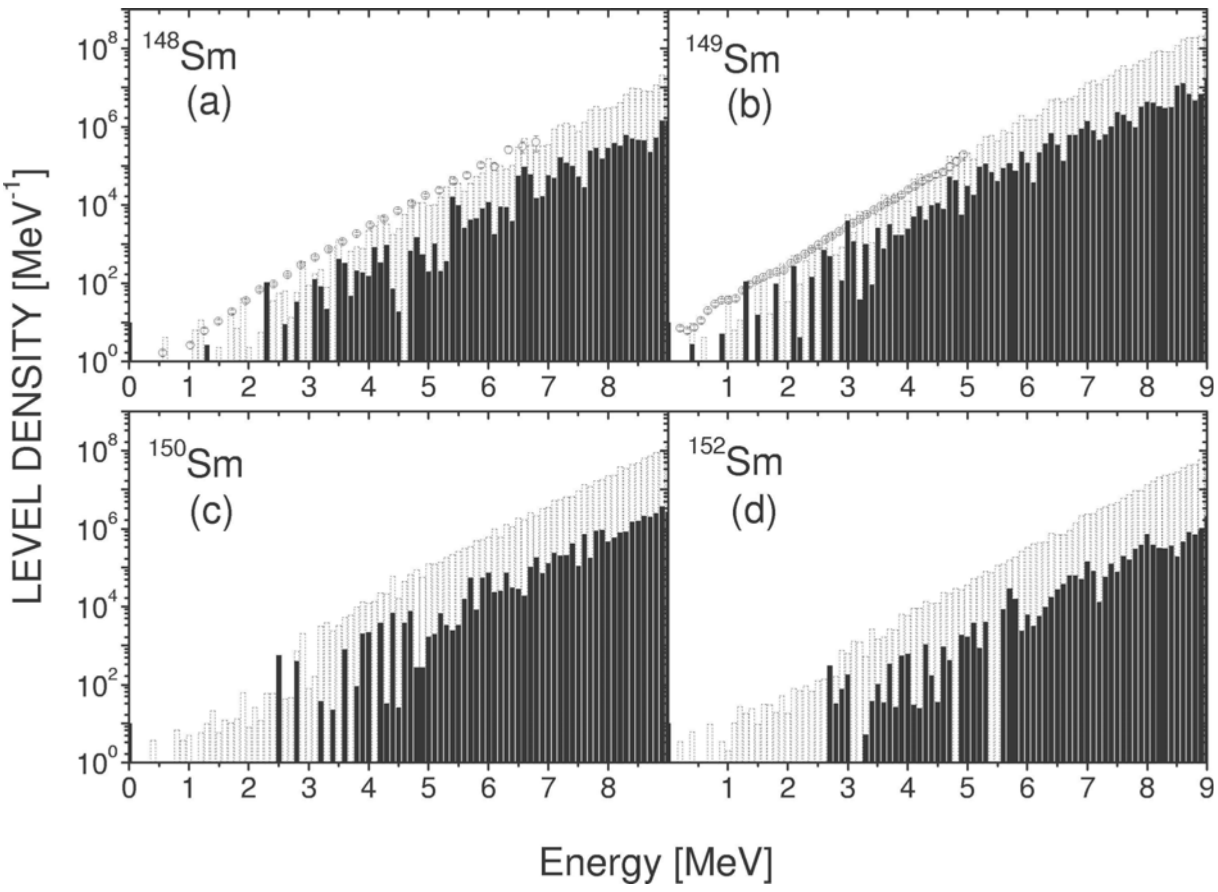

Fig. 1: Level densities (levels/MeV) of **^{148,149,150,152}Sm** vs. excitation energy (MeV): solid histograms: non-collective level densities; open histograms: total level densities; open circles: experimental data (S Siem *et al.,* Phys. Rev. C **65** (2002) 04318).

In addition to total level densities at $E < B_n$, the neutron binding energy, theoretical level densities of given angular momentum and parity *(J^{π})* around $E = B_n$, permit the evaluation of *s*- and *p*-wave neutron resonance spacings, D_0 and D_1 , respectively, in neutron radiative capture, to be compared with experimental data, in particular the accurate value of D_0 in neutron capture by **^{151}Sm**, leading to the compound nucleus **^{152}Sm**, measured recently by the n_TOF Collaboration at CERN (to be discussed in the next section).

Nuclear Reaction Theory and Experiments

Measurements of Neutron Cross Sections at the n_TOF Facility at CERN

After concluding the experimental campaign in 2004, 2005 has been dedicated to data analysis, in particular for the capture measurements, and to publication of technical papers, such as the description of the data acquisition system especially designed for the n_TOF facility [A.3], and review papers on the general characteristics of the facility and the cross section measurements of particular interest to the design of accelerator-driven systems [C.1].

The result of the first complete analysis of neutron radiative capture measured at n_TOF is the **^{151}Sm(n,γ)** cross section in the neutron energy range from 0.6 eV to 1 MeV, described in detail in a paper accepted in January 2006 for publication in Physical Review C. The measurement is relative to the **Au** standard, with an overall uncertainty of typically 6%.

The γ rays from capture events were detected with organic C_6D_6 scintillators and the data were analyzed by means of the pulse height weighting techique, suited to low-efficiency detectors, such as C_6D_6 , which, on the other hand, are only weakly affected by the background caused by neutrons scattered from the sample and captured by other materials in the experimental area. At low energies, resonances have been resolved up to about 1 keV, yielding a resonance integral of 3575 ± 120 b, an average *s*-wave resonance spacing of D_0 = 1.48 ± 0.04 eV (to be compared with a theoretical value of D_{0th} = 1.2 ± 0.1 eV from Ref. [A.2]), and a neutron strength function of $S_0 = (3.87 \pm 0.2) \cdot 10^{-4}$.

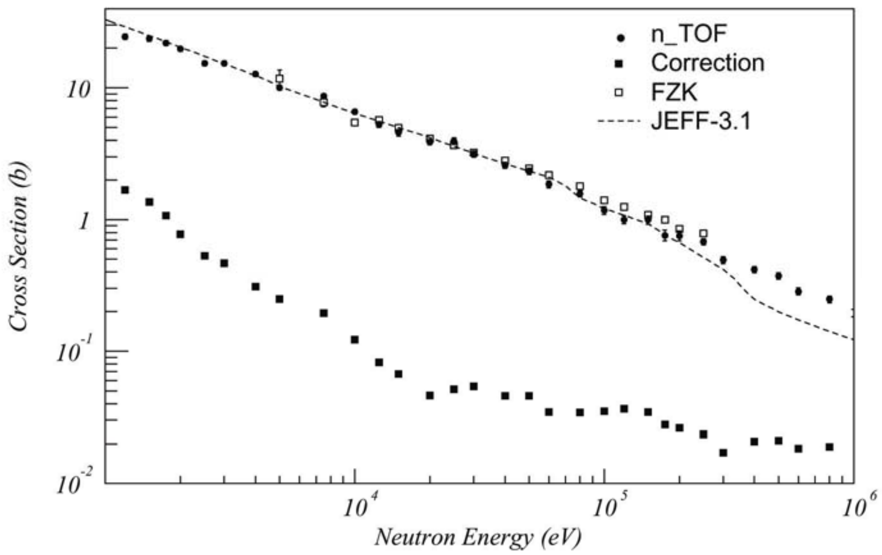

Fig. 2: **^{151}Sm(n,γ)** cross section in the unresolved resonance region. Solid dots: n_TOF measurements; solid squares: corrections for isotopic impurities, self-shielding and multiple scattering; open squares: experimental data of K. Wisshak *et al.*, Phys. Rev. C **73** (2006) 015802; dashed line: JEFF-3.1 evaluation.

The capture cross section in the unresolved resonance region is plotted in Fig. 2 as a function of neutron energy and compared with recent measurements carried out at the Forschungszentrum Karlsruhe (K. Wisshak *et al.*, Phys. Rev. C **73** (2006) 015802) and with evaluated data from the JEFF-3.1 library. Maxwellian-averaged capture cross sections are reported for thermal energies between 5 and 10 keV. In particular, the new value of the Maxwellian-averaged cross section at kT = 30 keV is 3.09 ± 0.15 b, considerably larger than previous theoretical estimates, thus providing better constraints for the thermodynamic conditions during the occurrence of the *slow* process in low mass stars in their asymptotic giant branch phase.

The second analysis already completed and submitted for publication concerns the ^{209}**Bi(n,γ)** cross section in the resolved resonance region. In the energy range from 0.8 to 23 keV four *s*- and 17 *p*-wave resonances were identified and their parameters compared with previous measurements performed at Oak Ridge and Geel. The n_TOF data of *s*-wave resonances show significant differences with respect to the corresponding Oak Ridge data, while better agreement is found with Geel measurements.

The third and last analysis refers to the ^{232}**Th(n,γ)** cross section in the unresolved resonance region, from 4 keV to 1 MeV. Fig. 3 shows $\sigma_{n\gamma}(E_n)\sqrt{E_n}$ as a function of neutron energy, E_n, in comparison with previous experimental data and a recent evaluation of ^{232}**Th** neutron cross sections up to 60 MeV carried out by R. Capote *et al.* as part of an IAEA coordinated research project. While there are significant discrepancies with some sets of previous experimental data, the agreement with the IAEA evaluation, performed before the n_TOF data became available, is excellent.

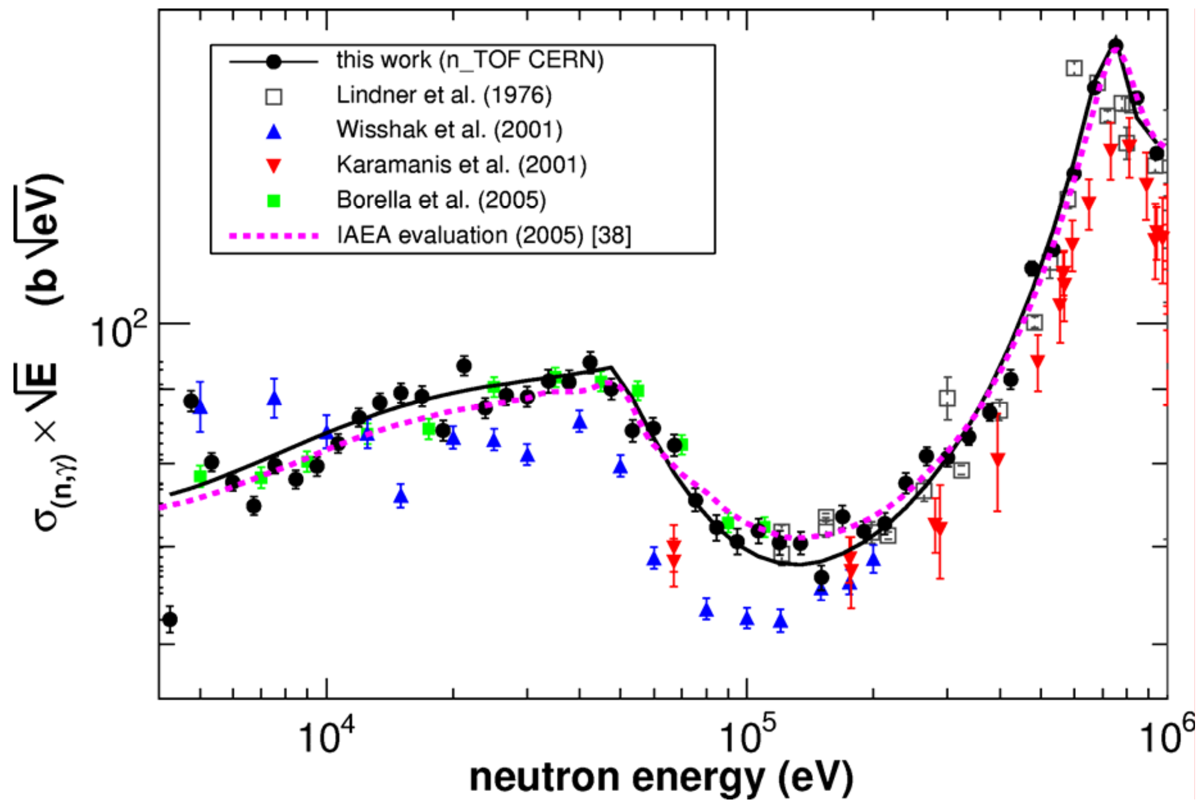

Fig. 3: $\sigma_{n\gamma}(E_n)\sqrt{E_n}$ vs. E_n for ^{232}**Th**, in comparison with previous experimental data and the IAEA evaluation by R. Capote *et al.* (to be published).

Finally, preliminary results on the ^{139}**La(n,γ)** cross section [C.2], the ^{204,206}**Pb(n,γ)** cross sections in the resolved resonance region [C.3] and neutron capture by ^{237}**Np**, ^{240}**Pu** and ^{243}**Am** [C.4] were presented at the 12th International Conference on Capture Gamma-Ray Spectroscopy and Related Topics, Notre Dame, Indiana, 5-9 September 2005.

$^{7}Li(n,\gamma)^{8}Li$ Reaction and Astrophysical S_{17} Factor at $E_{c.m.} > 500$ keV

Partial cross sections of neutron capture to the ground state and the first excited states of ^{8}**Li** have been measured in the neutron energy range from 10 to 80 keV [A.4]. By comparing the measured cross sections with calculations based on the direct capture mechanism, it has been shown that the cross sections are sensitive to the interaction potential of the incident neutron with the ^{7}**Li** target nucleus. This analysis permits a calculation, based on the same model of direct capture, of the astrophysical *S* factor for the ^{7}**Be(p,γ)**^{8}**B** reaction, S_{17}, in the continuum, at $E_{c.m.} > 500$ keV. The main reason for this approach is that direct measurements of the ^{7}**Be(p,γ)** reaction are affected by large uncertainties, due to the fact that ^{7}**Be** is radioactive and its proton capture cross section at energies of astrophysical interest is too low to be determined experimentally with current techniques.

Fig. 4 shows the ^{7}**Li(n,γ)** cross section measured in Ref. [A.4] in comparison with previous experimental data and direct capture model calculations.

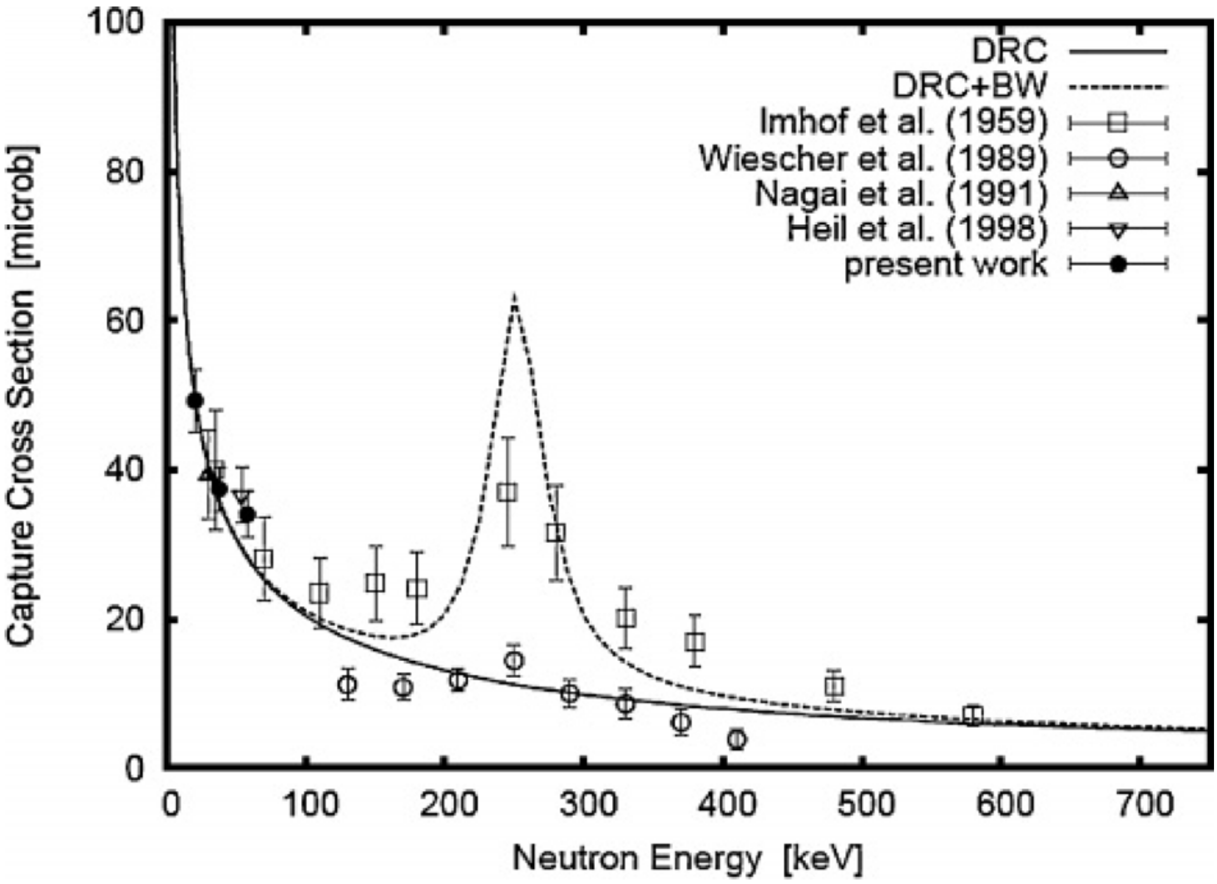

Fig. 4: ^{7}**Li(n,γ)** cross section vs. neutron energy. Solid dots: measurement of Ref. [A.4]. Solid line: direct capture model calculation. Dashed line: direct capture plus resonance capture in single-level Breit-Wigner approximation.

Stellar Capture Rates of ^{14}C

Neutron capture by ^{14}C plays a role in big bang nucleosynthesis, since, with its half-life of 5730 ± 40 years, ^{14}C can be considered as stable on the corresponding time scale and neutron capture by ^{14}C results in the production of heavier nuclei ($A > 20$).

In an experiment performed at Forschungszentrum Karlsruhe, the ^{14}**C(n,γ)**^{15}**C** cross section has been measured using the fast cyclic activation technique with averaged neutron energies of 30, 150 and 500 keV, and preliminary results have been published in Ref. [A.5].

Nuclear Data Processing and Validation

Cooperation of the Nuclear Data Group of the ENEA FIS-NUC Section with OECD/NEA Data Bank (Issy-les-Moulineaux, France) has continued, in particular, within the JEFF Working Group on Benchmark Testing, Data Processing and Evaluations.

The collaboration with specialists of the Russian research and development Institute of Physics and Power Engineering of Obninsk (IPPE-Obninsk) has also continued and been extended.

The activities concerning nuclear data processing, dedicated to production of cross-section libraries for neutron and photon transport calculations, were addressed to prepare libraries based on the new JEFF-3.1 European nuclear data file, officially released by the OECD/NEA Data Bank in May 2005.

As far as the production of pointwise (continuous-energy) cross-section libraries is concerned, a big effort was dedicated to producing a large multi-temperature library in ACE format for the American Monte Carlo code MCNP. In particular, through the NJOY-99.90 nuclear data processing system, all 381 JEFF-3.1 materials (isotopes and natural elements) were processed at 8 temperatures, typical of water-moderated thermal reactors and lead-cooled and sodium-cooled fast reactors. The specific library has been named MCJEFF31.BOLIB, and is presently under test and reporting.

As for the production of group cross-section libraries, a detailed feasibility analysis was concluded in order to verify the possibility of producing a coupled n-γ working library in FIDO format, similar, as much as possible, to the ENDFD/B-VI Rel. 3 BUGLE-96 American library, dedicated to LWR radiation shielding problems and related applications involving LWR pressure vessels and reactor internals dosimetry. The new library, characterized by the same energy group structure of BUGLE-96 (47 neutron groups + 20 photon groups), was collapsed with the SCAMPI nuclear data processing system from a multi-purpose fine-group cross-section library, based on JEFF-3.1. This “mother” library (VITJEFF31.BOLIB) was obtained with the NJOY-99.90 nuclear data processing system in the VITAMIN-B6 energy group structure (ENDF/B-VI Rel. 3 American library in AMPX format with 199 neutron groups and 42 photon groups), and was converted into the AMPX format with the SMILER module of SCAMPI. The new working library (BUGJEFF31.BOLIB) is specifically conceived for the deterministic discrete ordinates transport codes of the DOORS (ORNL) and DANTSYS (LANL) American systems. BUGJEFF31.BOLIB is in advanced state of development, and contains all the materials processed at infinite-dilution and several sets of cross sections self-shielded properly and weighted on specific neutron spectra of typical LWR mixtures of materials. The importance of this effort is linked, in particular, with the need of updated working libraries to be used with the three-dimensional discrete ordinates codes, like TORT (system DOORS) and THREEDANT (system DANTSYS). It is stressed that it is useful to generate updated working cross-section libraries for these codes, since they will increase our calculating capability in complex geometries if properly assisted by pre-post-processor programs for the automatic generation of spatial meshes and graphical verification of the geometrical model.

A collateral activity of response function data processing was performed in order to include in the future package of BUGJEFF31.BOLIB all available response functions obtained from the International Reactor Dosimetry File-2002 (IRDF-2002). In particular, all the dosimetry files contained in IRDF-2002 were collapsed to the 47 neutron energy group structure of the BUGLE-96 library by using the PREPRO 2004 American data processing system. The dosimetry cross-section collapsing was performed by starting from the 640 group-wise IRDF-2002 data file through the LINEAR and GROUPIE modules of PREPRO 2004 and from the point-wise IRDF-2002 data file by employing GROUPIE only. The collapsing process was performed using three weighting flux options: flat weight, ¼T PV (neutron spectrum at ¼T depth of a PWR pressure vessel) and a combination of three weighting functions (Maxwellian, 1/E and fission spectrum). A detailed report on this activity will be prepared in 2006.

Finally, a paper presented at the M&C 2005 International Topical Meeting in Avignon [C.5] describes the whole complex of activities addressed previously to the generation and validation of VITJEF22.BOLIB and MATJEF22.BOLIB fine-group libraries, respectively, in AMPX and MATXS format, based on the JEF-2.2 nuclear data file, processed in the VITAMIN-B6 energy group structure (199 neutron groups and 42 photon groups) and distributed by the OECD/NEA Data Bank.

Computer Code Development

BOT3P Code Package Development

BOT3P [A.6] is a set of standard FORTRAN 77 language codes, developed at the ENEA-Bologna Nuclear Data Group from August 1997. BOT3P gives the users of the deterministic transport codes DORT and TORT (both included in the Oak Ridge National Laboratory (ORNL-USA) DOORS package), TWODANT and THREEDANT (both included in the Los Alamos National Laboratory (LANL-USA) DANTSYS package), PARTISN (updated parallel version of DANTSYS) and the sensitivity code SUSD3D (distributed by OECD/NEA Data Bank (Issy-les-Moulineaux, France)), and some useful diagnostic tools to prepare and check the geometry of their input data files for both Cartesian and cylindrical geometries, including mesh grid generation modules, graphical display and utility programs for post-processing applications. For X-Y-Z TORT/THREEDANT/PARTISN mesh grids, BOT3P produces a geometrical input for the MCNP Monte Carlo transport code (LANL-USA) and also when the MCNP cells correspond to the X-Y-Z bodies created for TORT.

BOT3P stores the fine mesh arrays and the material zone map in a binary file, the content of which can be easily interfaced to any deterministic and Monte Carlo transport code. For example, the implementation of an interface in order to read this binary file has already been implemented for the KASKAD-S/KATRIN transport codes in the Keldysh Institute of Applied Mathematics (Moscow, Russia). Thus, users can potentially produce the geometrical and material distribution data for any transport code starting from the same BOT3P input. This makes it possible to compare directly for the same geometry the effects stemming from the use of different data libraries and solution approaches on transport analysis results.

All BOT3P versions let users model X-Y, X-Z, Y-Z, R-Θ and R-Z geometries in two dimensions and X-Y-Z and R-Θ-Z geometries in three dimensions.

BOT3P was successfully used not only in some complex neutron shielding and criticality benchmarks, but also in very large challenging problems such as for a power reactor application. Ansaldo Nucleare, Nuclear Division of Ansaldo Energia SpA, set up a R-Θ-Z geometrical model of about $2 \cdot 10^6$ meshes to calculate the internals heating rate distribution of the Westinghouse AP1000 reactor with TORT [R.1, C.6] by using BOT3P.

http://www.ansaldonucleare.it/TPap0305/NNPP/NPP_35.pdf

Through the use of BOT3P, radiation transport problems with complex 3D geometrical structures can be modelled much more easily, since a relatively small amount of engineer-time is required and refinement is achieved by changing few parameters.

BOT3P5.0 [R.2, C.7] is the latest version of the package and is designed to run on most Linux/UNIX platforms. It was released in the first half of 2005 and is publicly distributed by both OECD/NEA Data Bank [CC.1] and ORNL-RSICC [CC.2].

The main feature of BOT3P5.0 is the implementation of a general method to conserve the mass of the geometrically complex material zones simulated on both Cartesian and cylindrical mesh grids. BOT3P5.0 lets users optionally request as refined a computation as desired of the possible area/volume error of material zones due to the stair-cased geometry representation, and automatically corrects material densities in order to conserve masses globally. BOT3P5.0 can store on binary outputs the detailed material zone distribution map inside each cell of the mesh grid, according to a sub-mesh grid refinement defined in input by the user and the area/volume fraction distribution of the different material zones contained in meshes at zone interfaces. This also allows a local (per cell) density correction as an alternative to the approach of a uniform density correction on the whole zone domain, and potentially makes it possible to perform material zone homogenization locally and transport analyses with more accuracy.

Version BOT3P5.1 has been under development since summer 2005 and will be transferred to both the OECD/NEA Data Bank and ORNL/RSICC in 2006 for international distribution. In particular, the new additions will mainly be addressed to medical applications, in the terms of the activities carried out by the Computational Medical Physics Working Group (CMPWG), promoted and coordinated by the American Nuclear Society (http://cmpwg.ans.org/index.html). Particular attention will be devoted to the management of elaborated data coming from computerized axial tomography (CAT) scans in order to produce geometrical inputs suitable for transport analysis calculations.

The following plot is an example of the BOT3P complex modelling capabilities. It shows a XYZ mesh grid where three mutual orthogonal pipes of different radii intersect a sphere (volume conserved).

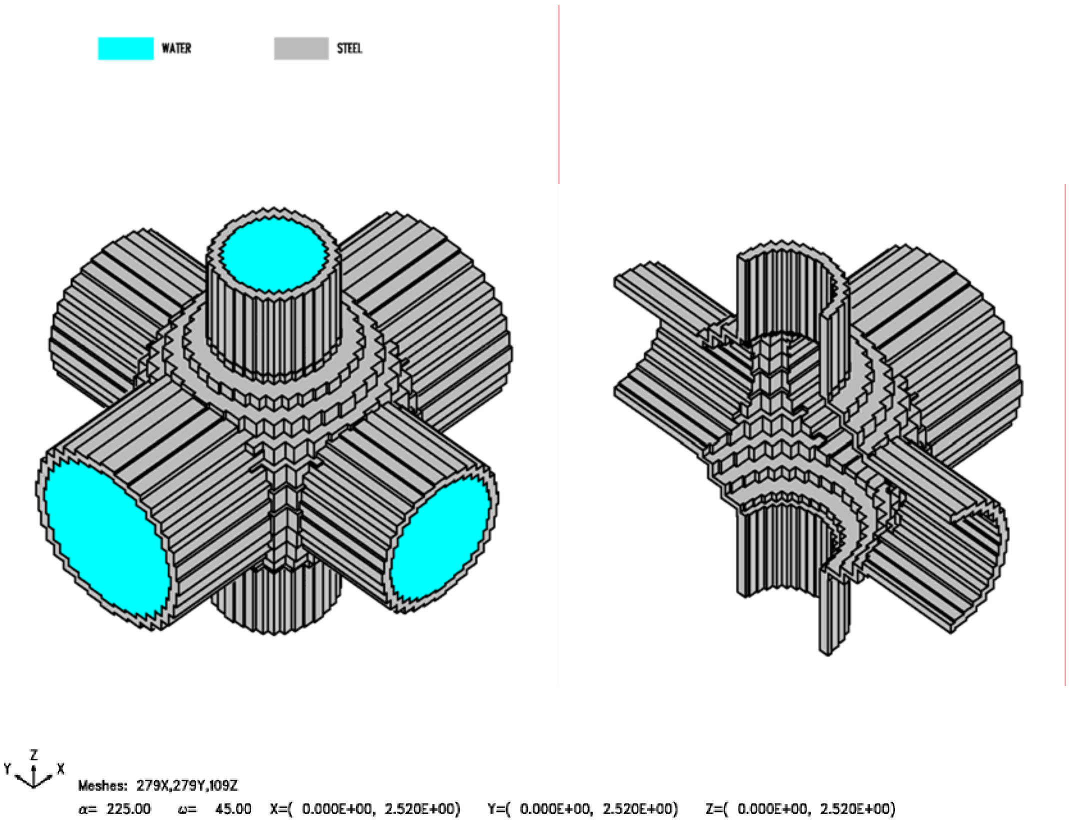

Fig. 5: Three Mutual Orthogonal Pipes with Different Radii Intersect a Sphere.

ADEFTA Version 3.0

ADEFTA (**A**tomic **De**nsities **f**or **T**ransport **A**nalysis) is a script file for any UNIX/Linux platform that uses only Bourne shell (bash) commands and the “awk” UNIX (and Linux) utility in order to calculate the atomic densities related to any compositional model for transport analysis. Moreover, ADEFTA is particularly directed towards users of both the GIP code, which prepares macroscopic cross sections for the DORT/TORT deterministic transport codes, and the MCNP Monte-Carlo code.

ADEFTA can run in Cygwin (http://www.cygwin.com), and so the output is available in Windows as well as in UNIX/Linux.

Version 3.0 [R.3] is different to Version 2.0, and accepts as input the partial weight or the weight percentage of each component of a material. Other minor updates make the use of ADEFTA more flexible with respect to the previous versions.

ADEFTA is publicly available from the OECD/NEA Data Bank [CC.3] and ORNL/RSICC, together with the BOT3P5.0 package [CC.2].

Publications of the Year 2005

Articles

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[A.5] R. Reifarth, M. Heil, R. Plag, U. Besserer, S. Dababneh, L. Dörr, J. Görres, R.C. Haight, F. Käppeler, A. Mengoni, S. O'Brien, N. Patronis, R.S. Rundberg, M. Wiescher and J.B. Wilhelmy, *Stellar Neutron Capture Rates of ^{14}C*, Nucl. Phys. A **758**, 787c-790c (2005).

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[C.2] R. Terlizzi and the n_TOF Collaboration, *Measurement of $^{139}La(n,\gamma)$ Cross Section,* CGS12, 12th International Conference on Capture Gamma-Ray Spectroscopy and RelatedTopics, Notre Dame, Indiana (USA), September 5-9, 2005.

[C.3] C. Domingo-Pardo and the n_TOF Collaboration, *Measurement of the Resonance Capture Cross Section of* ^{204,206}*Pb and Termination of the s-process,* CGS 12, 12th International Conference on Capture Gamma-Ray Spectroscopy and Related Topics, Notre Dame, IN (USA), September 5-9, 2005.

[C.4] D. Cano-Ott and the n_TOF Collaboration, *Neutron Capture Cross Section Measurements at n_TOF of* ^{237}*Np,* ^{240}*Pu and* ^{243}*Am for the Transmutation of Nuclear Waste, ,* CGS 12, 12th International Conference on Capture Gamma-Ray Spectroscopy and Related Topics, Notre Dame, IN (USA), September 5-9, 2005.

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