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Activity Report of the ENEA Nuclear Data Project in 2006

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March 2007

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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 2006.

March 2007

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General Quantum Mechanics

Scattering by PT-symmetric Non-local Potentials

Non-local potentials play an important role in many applications of quantum scattering theory. In nuclear physics, they naturally arise from the convolution of an effective nucleon-nucleon interaction with the density of a target nucleus.

In particular, a solvable non-local potential was proposed by Yamaguchi in 1954 in order to describe bound and scattering states of the proton-neutron system. We have studied in detail the scattering properties of a PT-symmetric one-dimensional version of the Yamaguchi potential, i.e., a non-Hermitian potential invariant under the product of the parity operator, P , and the time reversal operator, T , but not under the separate actions of P and T : the transmission and reflection coefficients are worked out by the Green's function method and show aspects of unitarity breaking quite different from those of PT-symmetric local potentials. The method of solution can be applied to large families of non-local potentials with separable kernel and different behaviour under P and T transformations [A.1].

Group Theory Approach to Transparent Potentials

One-dimensional potentials with transmission coefficient equal to one over the whole real axis occur in several domains of general quantum mechanics: for instance, non-trivial reflectionless potentials can be derived by supersymmetric techniques from the null potential, which is trivially reflectionless, or they can be extracted by Lie-algebraic methods from the Casimir invariants of some non-compact groups.

In our study [A.2], we have applied the latter technique to derive the general form of real potentials appearing in Hamiltonians with underlying $so(2,2)$ symmetry, which permits the solution of the corresponding Schrödinger equation in terms of hypergeometric functions. The six-generator $so(2,2)$ algebra admits several decomposition chains and the corresponding potentials are, in general, not transparent: reflectionless potentials are obtained in the $so(2,2) \rightarrow so(2,1) \rightarrow so(2)$ reduction chain when the solutions belong to the discrete series representations of the $so(2,1)$ sub-algebra appearing in the reduction. Hyperbolic potentials of the Pöschl-Teller type belong to this class.

The Inönü-Wigner contraction of $so(2,2)$ to the pseudo-euclidean algebra $e(2,1)$ yields solutions that are always connected with reflectionless potentials. For the sake of simplicity, but without loss of generality, we have worked out the general form of reflectionless potentials appearing in Hamiltonians with underlying $e(1,1)$ symmetry, where $e(1,1)$ is a three-generator sub-algebra of $e(2,1)$. The well-known reflectionless potential $V(x) \sim 1/x^2$ belongs to this class.

Nuclear Reaction Theory and Experiments

Neutron Induced Fission of Light Actinides

Within the work programme of theoretical activities of interest to the n_TOF Collaboration, we have proposed in Ref. [A.3] a model that describes the coarse-grained resonant structure in neutron induced fission of light actinides at sub-barrier excitation energies. The fission barriers are either two-, or three-humped, depending on the fissioning nucleus, and have an imaginary component in the second (isomeric) well, simulating a partial damping of class II vibrational states, while class III states, corresponding to excitations in the third well, are not damped. The sets of discrete transition states include rotational bands built either on vibrational states, or on non-collective states. In the present phenomenological version of the model, energies and quantum numbers of transition states are not evaluated by means of a nuclear structure model, but are adjusted on the experimental (n,f) cross sections, which can thus be reproduced with great accuracy, as shown in Figs. 1 and 2, relative to the first-chance fission of ^{232}Th and ^{231}Pa , respectively.

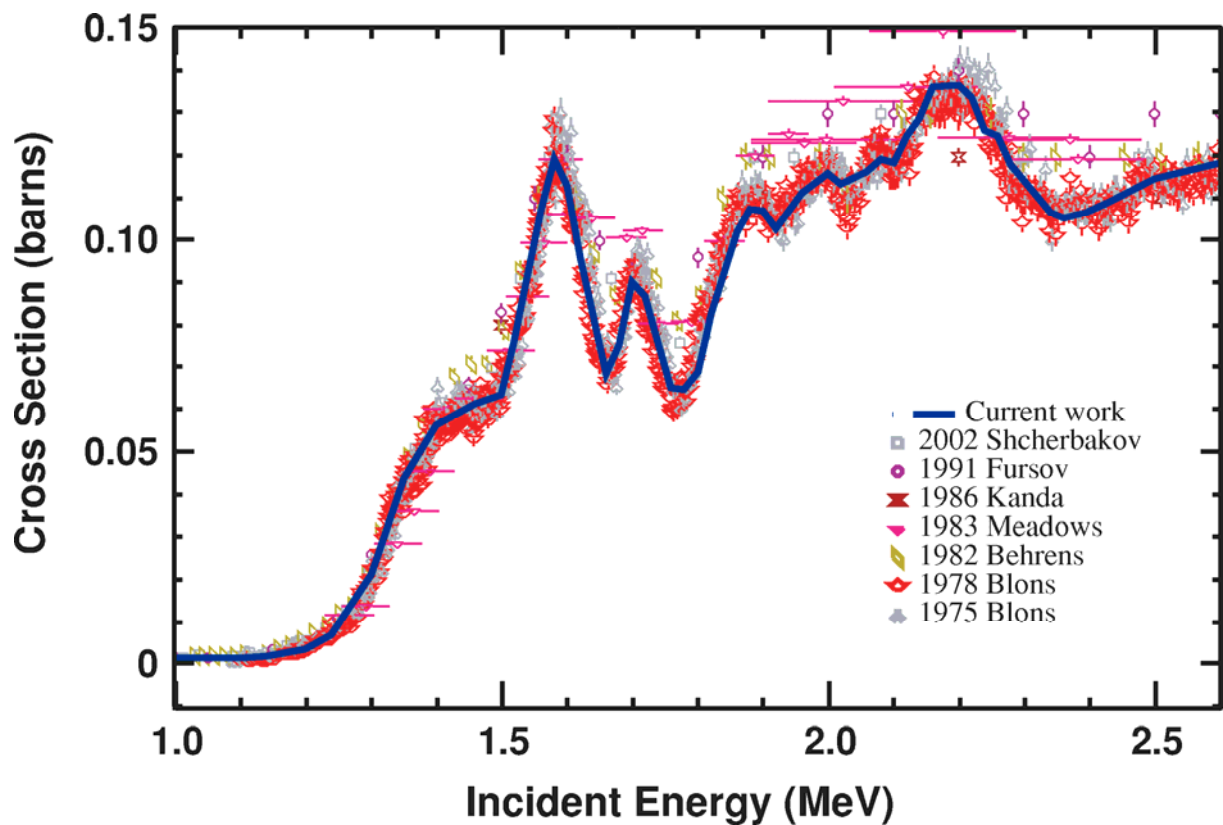


Fig. 1: $^{232}\text{Th}(n,f)$ near the fission threshold. Solid line: calculation from Ref. [A.3]. Experimental data are taken from EXFOR.

Our fission model has been incorporated in Version 19 (Lodi) of the EMPIRE-II code of nuclear reactions, freely distributed by the National Nuclear Data Center, Brookhaven National Laboratory.

The fission calculations for ^{232}Th and ^{231}Pa are part of a series of evaluations of neutron cross sections of the above mentioned isotopes undertaken within a research project coordinated by the IAEA Nuclear Data Section.

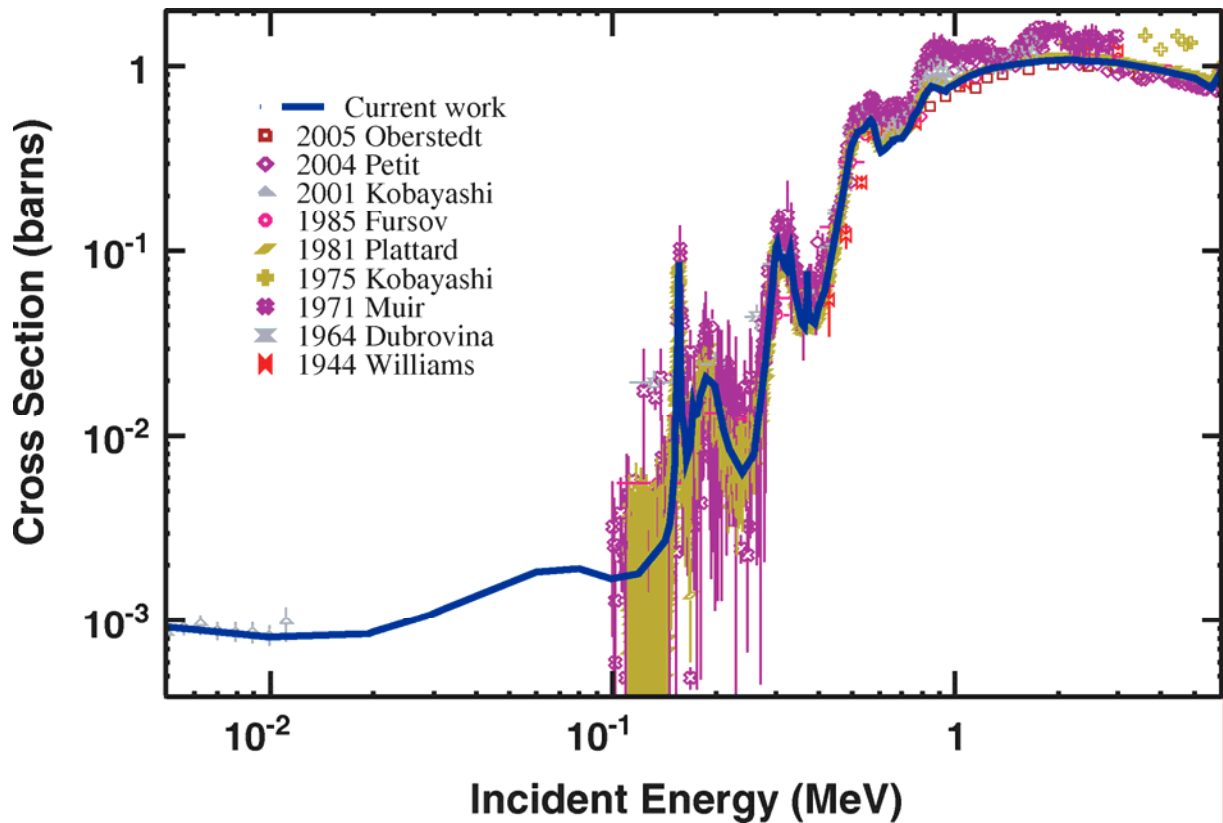


Fig. 2: $^{231}\text{Pa}(n,f)$ in the neutron energy range from 5 keV to 5 MeV. Solid line: calculation from Ref. [A.3]. Experimental data are taken from EXFOR.

Measurements of Neutron Capture Cross Sections at the n_TOF Facility at CERN

At the end of the experimental campaign in 2004, the two subsequent years have been dedicated to the analysis of capture cross section measurements, and to publication of related papers, such as those on $^{232}\text{Th}(n,\gamma)$ in the unresolved resonance region up to 1 MeV [A.4], $^{151}\text{Sm}(n,\gamma)$ in the energy range from 0.6 eV to 1 MeV [A.5], and $^{209}\text{Bi}(n,\gamma)$ in the resolved resonance region [A.6], already summarized in the 2005 activity report.

The new analysis completed and published in 2006 concerns the $^{207}\text{Pb}(n,\gamma)$ reaction in the resolved resonance region [A.7]. The measurement has been performed with an optimized set up of two C_6D_6 scintillator detectors, which permits reduction of scattered neutron background down to a negligible level, by using the pulse height weighting technique. Resonance parameters and radiative kernels have been determined for 16 resonances in the neutron energy range from 3 keV to 320 keV. Good agreement with previous measurements is found at low energies, while substantial discrepancies appear beyond 45 keV. Maxwellian averaged cross sections have been determined with an accuracy of $\pm 5\%$.

Preliminary results from analysis of neutron capture by other isotopes have been presented at various conferences, such as the 9th International Symposium on Nuclei in the Cosmos (NIC-IX), CERN, Geneva, 25-30 June 2006 [C.1-5] and the American Nuclear Society's Topical Meeting on Reactor Physics (PHYSOR-2006), Vancouver, Canada, 10-14 September 2006 [C.6-8].

Nuclear Data Processing and Validation

The cooperation between the ENEA Nuclear Data Group and the OECD/NEA Data Bank (Issy-les-Moulineaux, France) continued, in particular, within the JEFF Working Group on Benchmark Testing, Data Processing and Evaluations. In particular, several feedbacks were notified dedicated to the JEFF-3.1 European evaluated data files and their related processing through the NJOY nuclear data processing system.

The collaboration with V. Sinitsa (Obninsk) has continued and been extended.

VITJEFF31.BOLIB and MATJEFF31.BOLIB

The VITJEFF31.BOLIB and MATJEFF31.BOLIB coupled n- γ multi-group cross section libraries for nuclear fission applications in the VITAMIN-B6 American library energy group structure (199 neutron groups + 42 photon groups) were completely reprocessed by means of a version of the NJOY-99.112 nuclear data processing system modified at ENEA, Bologna. The present libraries, based on the JEFF-3.1 European evaluated nuclear data files, were previously produced in Bologna through the NJOY-99.90 system, but it was decided to reprocess them completely after a detailed analysis of the list of modifications introduced by the author in the recent NJOY-99.112 version. The THERMR and GROUPR modules of this latter version were further modified at ENEA-Bologna. In particular, a correction patch was prepared and introduced in the THERMR module of NJOY-99.112 in order to solve a problem emerged in the processing of the JEFF-3.1 bound nuclides C (graphite) and Be (beryllium metal), where infinite loop calculations were generated.

A second relevant correction patch was prepared by Sinitsa in Bologna for the GROUPR module of NJOY-99.112. The OECD/NEA Data Bank checked this patch with positive results and then diffused it freely. This initiative was taken in Bologna in order to extend the group-wise data processing capability to the evaluated data files including non Cartesian interpolation schemes for secondary neutron energy distributions (MF = 5).

Our efforts revealed that 69 JEFF-3.1 evaluated files could not be processed correctly through the GROUPR module of NJOY-99.112 or through all previous NJOY versions officially released, as communicated by ENEA-Bologna to the NJOY User Group. This set of data files contains, in particular, secondary neutron energy distributions (MF=5), presented as arbitrary tabulated functions (LF = 1) with the non Cartesian unit base interpolation law INT=22. The GROUPR module cannot process correctly the mentioned evaluated files because the GETSED subroutine cannot deal with secondary neutron energy distributions with non Cartesian interpolation schemes (INT = 11-15 and INT = 21-25). Thus, the group-to-group scattering matrices for the MT=16, 17, 22, 28, 32, 33, 91 reactions could not be produced in the GENDF output cross section files of the 69 evaluated data files under consideration.

The GROUPR problems described above were autonomously identified in Bologna, starting from the analysis of unacceptably underestimated K_{eff} results obtained with criticality neutron transport calculations, performed through the XSDRNPM one-dimensional (1D) discrete ordinates module of the SCAMPI data processing system. Two ICSBEP (2004 Version) fast criticality benchmark experiments with ^{233}U (included in the previously cited 69 file set) were simulated. The results obtained with the XSDRNPM code in the P5-S16 approximation were obtained from JEFF-3.1 data, processed differently with the original GROUPR module of NJOY-99.112 and with the GROUPR version modified at ENEA into the 199 neutron energy group structure of the VITAMIN-B6 library. The results obtained with these deterministic

transport calculations were compared with the results obtained through the MCNP-4C Monte Carlo code using JEFF-3.1 continuous energy cross section sets.

181 materials were processed: 175 materials for standard isotopes or natural elements and 6 materials for bound nuclides. In this last group of materials, in particular, the H-Zr material was added to the 5 materials of bound nuclides contained in the VITAMIN-B6 library.

Only one material (^{46}Ca from JEFF-3.1) could not be processed correctly, but recently the OECD/NEA Data Bank distributed a revised version of this file, produced by the original author. ENEA-Bologna notified the OECD/NEA Data Bank that the total and elastic cross section values of the first officially released version of this ^{46}Ca file below 1 keV, i.e. in the energy range $1.0\text{E}-05$ - $1.0\text{E}+03$ eV, are set to zero, while capture cross section values differ from zero.

SCAMPI Revision and Updating

Many corrections and modifications to several modules of the SCAMPI data processing system were required in order to process the JEFF-3.1 data for the VITJEFF31.BOLIB library. In particular, the AJAX, MALOCS and SMILER modules were corrected. A detailed list of the actions performed is presented in the dedicated table

The following versions of the MALOCS module were compared, as taken from the SCAMPI nuclear data processing and SCALE nuclear safety calculation systems:

- a) Original version of MALOCS in the SCAMPI distributed by the NEA Data Bank;
- b) MALOCS/SCAMPI-Bologna version modified by Sinitsa;
- c) Original version of MALOCS included in SCALE-4;
- d) Original most recent updated version of MALOCS included in SCALE-5.

From the performance and feature comparison of the versions of MALOCS included in the SCAMPI, SCALE-4 and SCALE-5 systems, the following conclusions were drawn:

MALOCS/SCAMPI, MALOCS/SCALE-4 and MALOCS/SCALE-5 exclude the possibility of fission matrix collapsing.

MALOCS/SCALE-4 and MALOCS/SCALE-5 include the possibility to truncate the up-scatter cross section terms with options IOPT7 = 0, 1, 2, 3.

MALOCS/SCAMPI includes only IOPT7 = 0.

MALOCS/SCALE-5 is similar to MALOCS/SCALE-4, but it is rewritten in Fortran-90.

MALOCS/SCAMPI-Bologna, includes the possibility of fission matrix collapsing and permits truncation of the up-scatter terms with options IOPT7 = 0, 1, 2, 3.

Taking into account both these conclusions and the fact that the SCAMPI system includes functional modules all programmed in FORTRAN-77 as the MALOCS/SCAMPI Bologna version, we preferred avoiding any potential inconsistency in programming languages; therefore, this version was selected for the production of the new BUGJEFF31.BOLIB collapsed working library from the multi-group general-purpose VITJEFF31.BOLIB library in AMPX format.

SCAMPI Updating and Corrections

N	JEFF-3.1 Materials	Error Message	Problem	Modules Modified
1.	H-3 He-4	“floating invalid” SCAMPI run stopped	Cross-section MT=102 (n,γ) is absent in the evaluations but is required by SMILER - necessary to bypass this possibility.	SMILER/fixsum
2.	Al-27 Cl-35	“requires too much data” SCAMPI run stopped	Number of reaction types exceeds the maximum allowed number (100) - necessary to increase value.	AJAX/ann MALOCS/lapser MALOCS/cflux
3.	Sn-117 Eu-152 Eu-153 Pu-238	“floating invalid” SCAMPI run stopped	Scattering matrices MF=6 MT=91 for moments l=1, 3, 5 ... are equal to zero - necessary to correct the structure of the AMPX record presentation in order to include the possibility to describe matrices with all elements equal to 0.	SMILER/comp
4.	Ca-40 Ca-42 Ca-44 Ti-49 Fe-58 Pb-206 Pb-207 Pb-208	“floating invalid” SCAMPI run stopped	Numerical data in scattering matrices with very small values ($\leq 10^{-31}$) appear as a result of double-precision calculations, and must be set to 0.	SMILER/froggy
5.	Fission matrices for fissile nuclides; photo- atomic cross- sections for all nuclides	No diagnostic	The most recent versions of NJOY (starting from NJOY-97) present the cited data in different formats (fixed point and exponential notation) and SMILER can only read data correctly in exponential notation, so it was necessary to change the reading format.	SMILER/rgendf
6.	Fissile nuclides	No diagnostic	SMILER can only read the prompt component (MF=6 and MT=18) of the total fission spectrum needed for fixed source transport calculations - necessary to modify SMILER and MALOCS in order to take into account the delayed component part (MF=5 and MT=455).	SMILER/rgendf SMILER/master SMILER/chi1d MALOCS/avg1

The GENDF cross section files, obtained through a modified version of GROUPR in NJOY-99.112, were used to generate VITJEFF31.BOLIB and MATJEFF31.BOLIB. Extensive validation of the VITJEFF31.BOLIB library was performed through the simulation of the same thermal and fast neutron criticality benchmarks, already prepared for VITJEF22.BOLIB. The results obtained with the XSDRNPM one-dimensional transport module of SCAMPI were compared with the results of Monte Carlo calculations using the MCNP-4C code.

BUGJEFF31.BOLIB

Two preliminary versions (with and without up-scatter) of the cross section working library called BUGJEFF31.BOLIB were collapsed from the VITJEFF31.BOLIB library in AMPX format, processed with our modified version of NJOY-99.112. This work was done by means of the ENEA-Bologna revised SCAMPI system and, in particular, the modified version of the MALOCS module. The BUGJEFF31.BOLIB working library for shielding and LWR pressure vessel dosimetry applications has the same group structure (47 n + 20 γ) and general features as the BUGLE-96 American library.

In order to complete the response function cross section collapsing in the BUGLE-96 neutron group structure (47 n) from the most recent IAEA Reactor Dosimetry File IRDF-2002, a new tabulated weighting function was obtained from XSDRNPM calculations in the 1/4 T PWR-PV position, using the VITJEFF31.BOLIB multigroup library.

The calculational chain was completely prepared but, before starting the collapsing procedure for the generation of the final working library, further examination will be necessary to identify the inconsistencies and inaccuracies of the the BUGLE-96 input data, emerged in 2005 in the ENEA feasibility analysis for a BUGLE-type library generation.

Computer Code Development

BOT3P is a set of standard FORTRAN 77 language codes developed at the ENEA Nuclear Data Group as from August 1997.

BOT3P Version 1.0 was originally conceived as a set of standard FORTRAN 77 language programs in order to give the users of the DORT and TORT deterministic transport codes (both included in the Oak Ridge National Laboratory (ORNL-USA) DOORS package) some useful diagnostic tools to prepare and check their input data files for both Cartesian and cylindrical geometries, including mesh grid generation modules, graphical display and utility programs for post-processing applications. Later versions extended the possibility to produce the geometrical, material distribution and fixed neutron source data to other deterministic transport codes such as TWODANT/THREEDANT (both included in the Los Alamos National Laboratory (LANL-USA) DANTSYS package), PARTISN (the updated parallel version of DANTSYS) and the sensitivity code SUS3D (distributed by OECD/NEA Data Bank (Issy-les-Moulineaux, France) and, potentially, to any transport code through BOT3P binary output files that can be easily interfaced (see, for example, the case of the two-dimensional (2D) and three-dimensional (3D) discrete ordinates neutron, photon and charged particle transport codes KASKAD-S-2.5 and KATRIN-2.0, developed in the Keldysh Institute of Applied Mathematics (Moscow, Russian Federation)). Moreover, in the case of X-Y-Z TORT/THREEDANT/PARTISN mesh grids, BOT3P also produces a geometrical input for the MCNP Monte Carlo transport code (LANL-USA), where the MCNP cells correspond to the X-Y-Z bodies created for TORT. Since BOT3P binary output files can be easily

interfaced, 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.

BOT3P Version 5.1 [R.1, R.2] was completed in 2006 and is freely available from OECD/NEA Data Bank (F) since August 2006 (<http://www.nea.fr/abs/html/nea-1678.html>). BOT3P Version 5.0 is distributed by ORNL-RSICC (USA) (<http://rsicc.ornl.gov/codes/psr/psr5/psr-530.html>). BOT3P Version 5.1 contains important additions specifically addressed to radiation transport analysis for medical applications. The new module CATSM [R.3] allows users to reduce the geometrical size of problems related to elaborated (already interpreted by physicians or by proper software) computerized (axial) tomography (CT/CAT) scans without or with small detail loss with respect to the original voxelized geometry. This permits problem sizes that can be more easily managed by transport codes. CATSM can automatically generate tetrahedron mesh grids too, starting from the input voxelized geometry, even though the implemented algorithm is still rather rough and to be improved in the future. BOT3P-5.1 contains new graphics capabilities that enable users to visualize tetrahedron mesh grids in 3D and 2D cuts.

As from Version 5.0, a general method to conserve mass of geometrically complex material zones simulated on both Cartesian and cylindrical mesh grids was implemented [A.8]. BOT3P allows users to specify 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. BOT3P 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 procedure 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 homogenisation locally and transport analyses with more accuracy.

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

BOT3P was developed on a DIGITAL UNIX ALPHA 500/333 Workstation and was successfully used not only in some complex neutron shielding and criticality benchmarks [A.9], but also in power reactor applications (Westinghouse AP1000 internals heating rate distribution calculations by Ansaldo Nucleare (Italy) [A.10]). BOT3P was also tested on Red Hat Linux 7.1 and OpenSUSE 10.2 and is designed to run on most UNIX platforms.

The following plots give an idea of the BOT3P complex modelling capabilities.

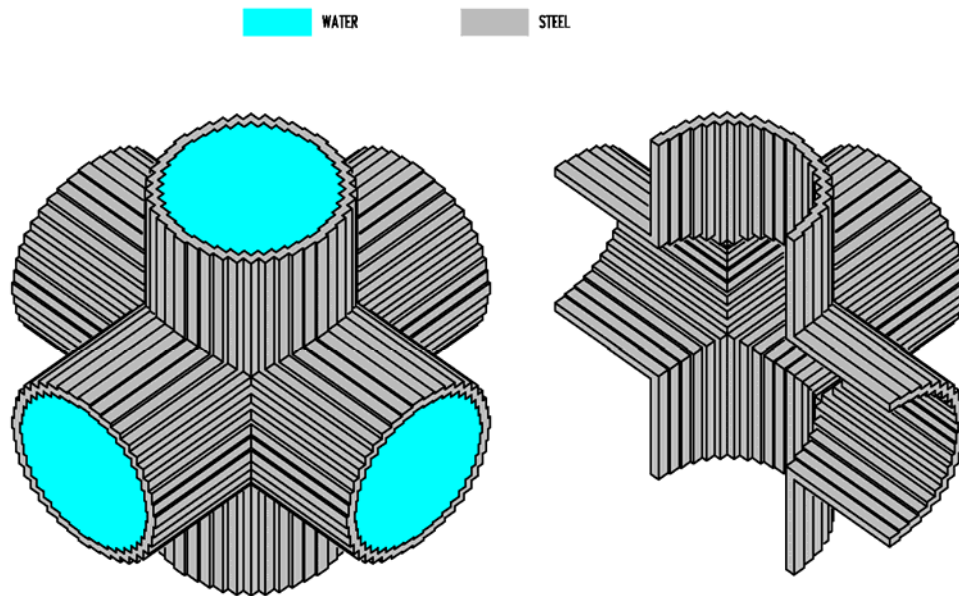


Fig. 3: Cartesian grid (45X, 45Y, 45Z) of three mutual orthogonal pipes of the same radius.

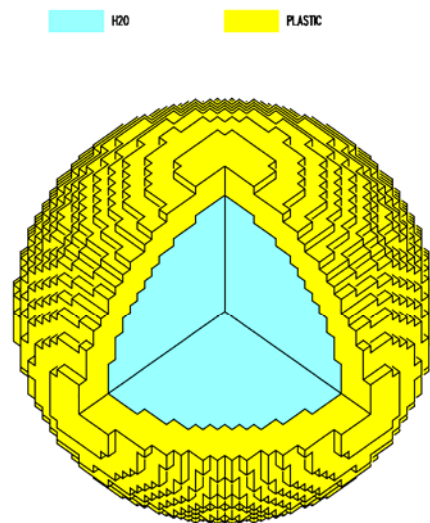


Fig. 4: Cut-away of a Cartesian grid (40X, 40Y, 40Z) reproducing a spherical object.

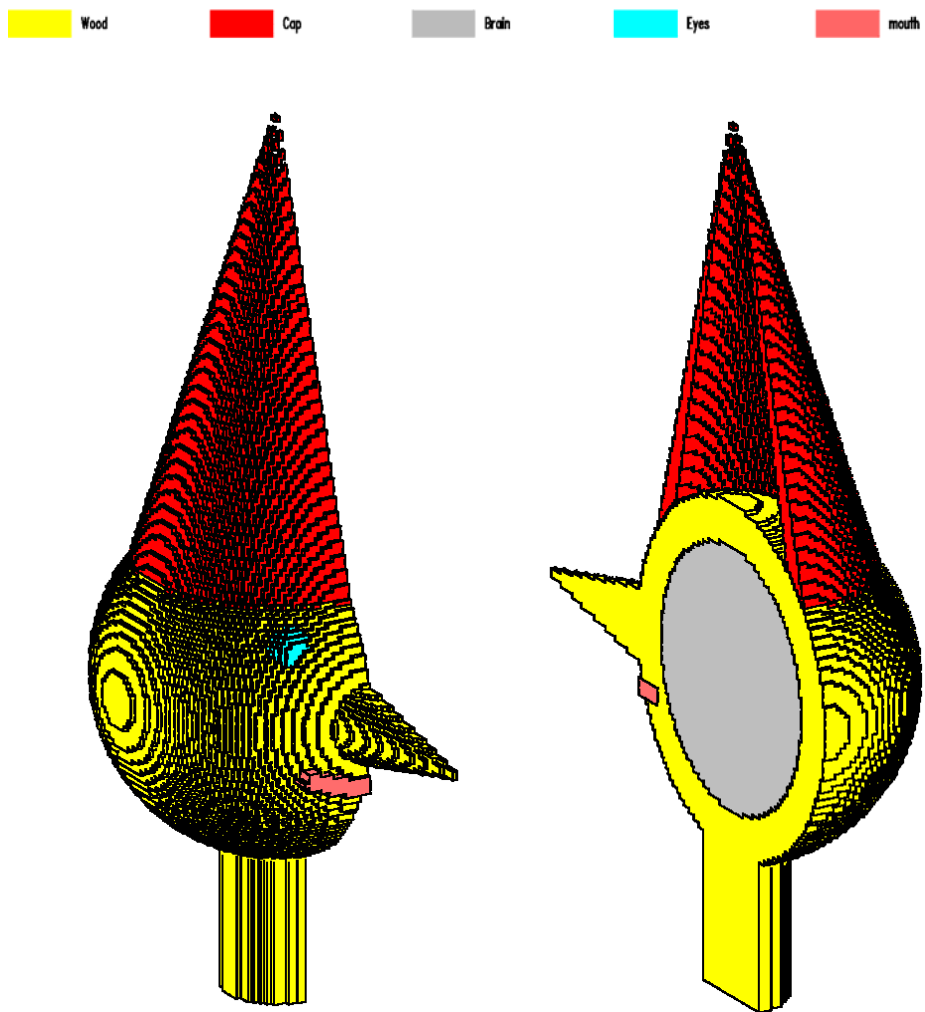


Fig. 5: Simulation in Cartesian Co-ordinates of a Complex Geometry (120X, 88Y, 200Z)

Publications 2006

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- [A.1] F. Cannata and A. Ventura, *Scattering by PT-symmetric Non-local Potentials*, Czech. J. Phys. **56**, 943-951 (2006).
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- [C.1] M. Heil *et al.* (the n_TOF Collaboration), *Neutron Capture Cross Section Measurements for Nuclear Astrophysics at n_TOF*, Proceed. of the 9th Int. Symp. on Nuclei in the Cosmos (NIC-IX), CERN, Geneva, 25-30 June 2006, SISSA Proceedings of Science (<http://pos.sissa.it/>), PoS (NIC-IX) 053.
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