Transactions

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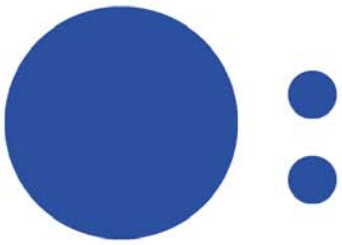
NUCLEAR ENGINEERING SCIENCE AND TECHNOLOGY



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NUCLEONICA Web Portal

NUCLEONICA:
A WEB PORTAL FOR THE NUCLEAR SCIENCES

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ABSTRACT

NUCLEONICA (www.nucleonica.net) is a new nuclear science web portal from the European Commission's Joint Research Centre. The portal provides a customisable, integrated environment and collaboration platform for the nuclear sciences using the latest internet "Web 2.0" technology. NUCLEONICA is aimed at professionals, academics and students working in fields as diverse as the life and earth sciences, and the more traditional disciplines such as nuclear power, health physics and radiation protection, nuclear and radio-chemistry, and astrophysics. It is also used as a knowledge management tool to preserve nuclear knowledge built up over many decades by creating modern web-based versions of so-called "legacy" computer codes. All NUCLEONICA's web applications are browser and operating system independent and can be accessed by a variety of mobile devices.

1. Introduction

Education, training and knowledge management in the nuclear field require the renaissance of sophisticated computational skills and tools which support recent developments on issues such as energy security and protection of the environment, advanced nuclear fuel cycles, qualitative and quantitative analyses of future nuclear power growth scenarios etc. The new nuclear science web portal NUCLEONICA contributes to this skill renaissance by offering many features which encompass the knowledge of generations of nuclear scientists.
NUCLEONICA is the latest development in a family of information systems for the nuclear science community. From the software technical point of view the history began with Nuclides 2000 [1] (a classical client side database application), developed further to Nuclides.net which was a combination of local client side database connected with web-based application modules. The most recent member of the family, NUCLEONICA [2], is fully web-based requiring, on the client side, only a web browser and internet access [3]. The NUCLEONICA portal (Fig 1) consists of four main "Centres" (Fig 2): Data Centre, Application Centre, Knowledge Centre, and Networking Centre.

2. Data Centre

Nuclear data can be accessed through online interactive nuclide charts [4] (based on decay modes, half-lives, binding energy, spin, parity, etc.), reference data (datasheets, derived data, cross sections, spectral data, fission yields, etc.) and searchable databases for internationally evaluated nuclear data. The NUCLEONICA database [1], which is based on the Joint Evaluated Fission and Fusion (JEFF3.1) radioactive decay datafile, contains decay data on 3896 nuclides in ground and isomeric states. In addition, spectral data with a total of approximately 54000 energies and emission probabilities is available. Additional databases include the 8th Table of Isotopes, prompt gamma neutron activation data, and effective dose coefficients.

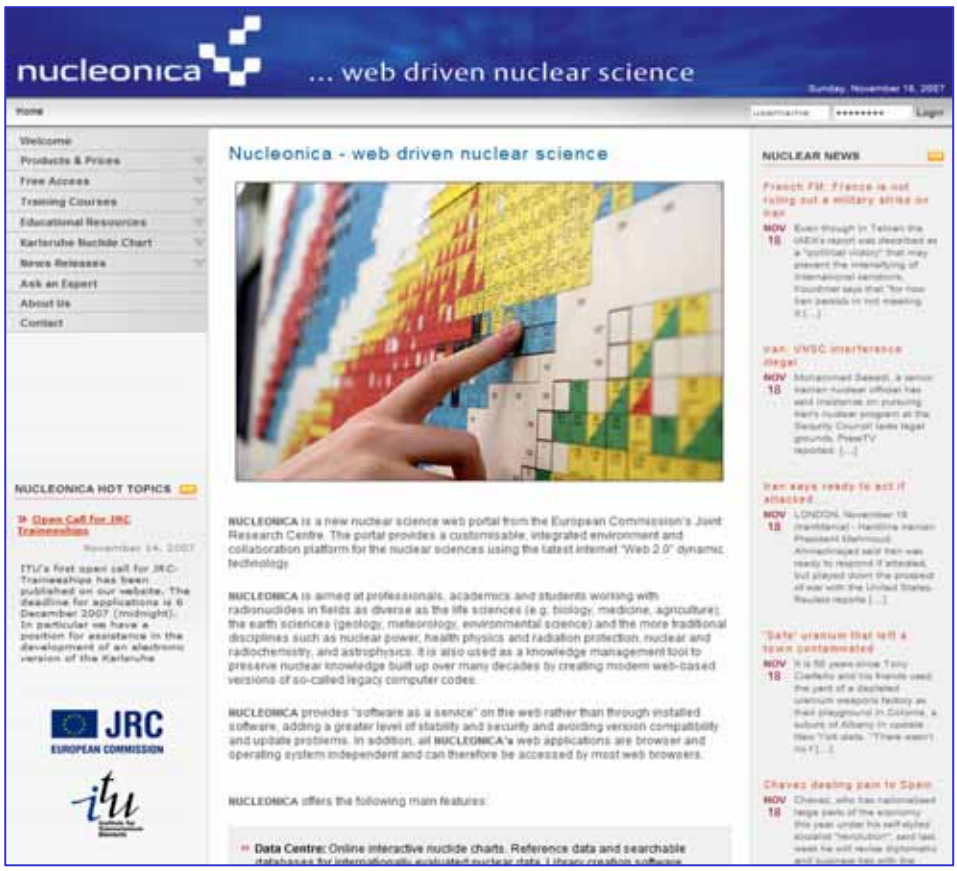

Fig 1. NUCLEONICA nuclear science portal.

3. Applications Centre

NUCLEONICA applications are designed to be user friendly, intuitive, and require a minimum of learning time. These powerful applications, which form the “backbone” of the nuclear science portal, can be used by professionals and students for everyday calculations. For advanced users, NUCLEONICA provides a more “hands-on” approach with its advanced scripting interface [5].

The application modules include radioactive decay, dosimetry & shielding [6], fission yields, transport and packaging, library creation for spectroscopy, nuclide mixtures, webGraphics. Recently added applications include a range and stopping power module for charged particle interaction with matter (collaboration with Ondokuz Mayis University) [7] and a radiological dispersion module for collective dose estimates following a radiological dispersion event (restricted access). Currently a new gamma spectrum simulator for a wide range of NaI and HPGe detectors is under development [8].

Through a collaboration between the Karlsruhe Research Centre and the Institute for Transuranium Elements, a web-based version of KORIGEN called webKORIGEN [9] has been developed for use in NUCLEONICA. For users, webKORIGEN overcomes the necessity of installation, input preparation and processing, compilation and debugging by offering an intuitive user-friendly web-based application – ideal for training purposes. With webKORIGEN, the user can concentrate on science rather than on the technicalities of large Fortran computer codes. WebKORIGEN supports calculations for a set of standardized problems, trimmed to three major classes of nuclear plants: the thermal power plants deployed worldwide as Pressurized Water Reactors (PWR) and Boiling Water Reactors (BWR) and a future extension to the current industrial technology the European Fast Reactor (EFR). This is discussed in more detail in section 6 in the context of preservation of nuclear knowledge and as an example of the development of a web application from a legacy computer code.

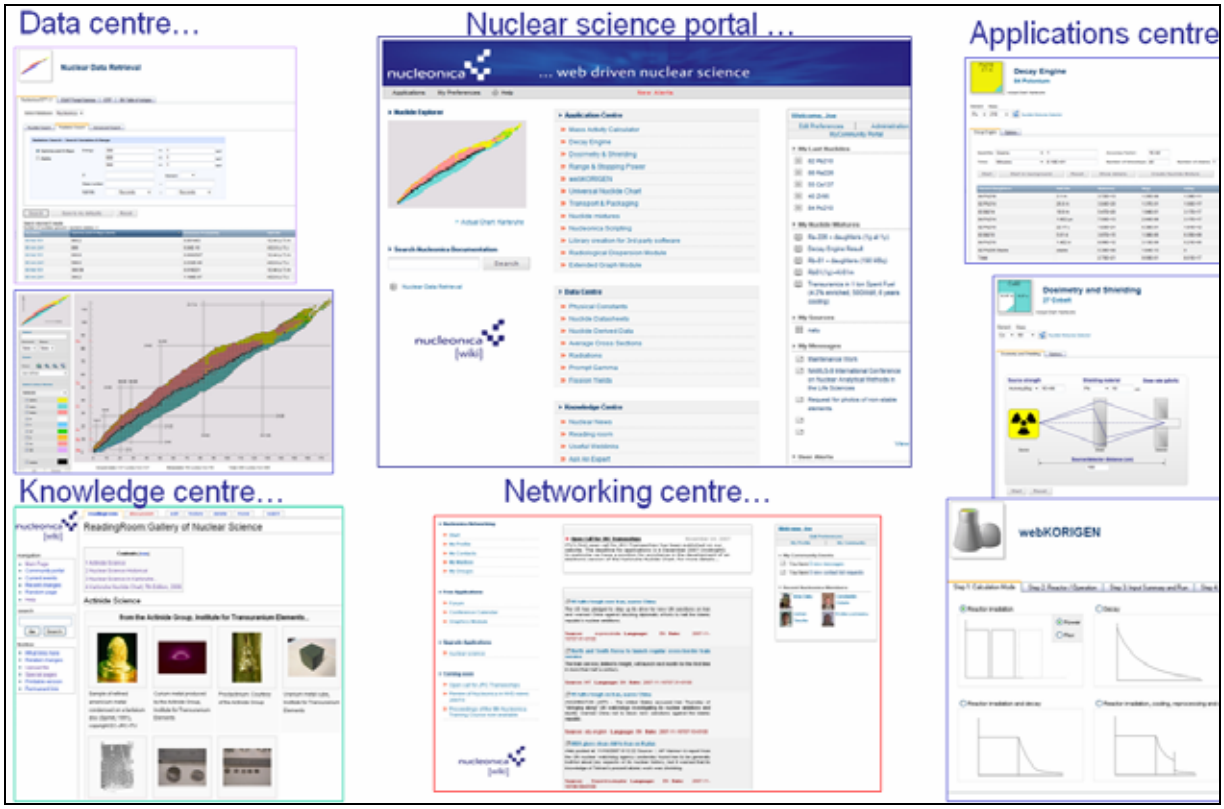

Fig 2. NUCLEONICA's main "Centres" for Data, Applications, Knowledge and Networking.

4. Knowledge Centre

The *Knowledge Centre*, or NucleonicaWiki [10], is the content management system (CMS) used for NUCLEONICA documentation. It is based on the same MediaWiki "engine" as used in Wikipedia. The NucleonicaWiki is used for online Help, ReadingRoom (for articles, and presentations), weblinks, element information, ask an expert Q & A etc.
The NucleonicaWiki is also used for training course organisation. To date, nine nuclear science training courses based on Nucleonica have taken place both at ITU and in external training centres. All training course announcements [11], agendas, full presentations, exercises, case studies, photo galleries etc., are available online in the NucleonicaWiki. NUCLEONICA training courses introduce the basic concepts of nuclear science and technology and are suitable for participants from the nuclear industry, nuclear research organizations, universities, regulatory authorities etc. Lectures are followed by “hands-on” case studies on the use of the NUCLEONICA web-based applications.
In addition to the above described nuclear science training courses, in 2008 we plan to initiate a number of short-stay training activities on NUCLEONICA at ITU. These short-stay training courses will provide PhD students, research fellows and trainees with a more extensive training in the use of NUCLEONICA through "mini-projects". Calls for proposals for such "mini-projects" will be announced on the NUCLEONICA website.

5. Networking Centre

The *Networking Centre* allows users to stay in contact with colleagues from workshops or conferences, meet scientists from similar areas of interest and build up an international contact list. The users can represent themselves (personal page) and their Institute/Organisation in the international science community. The nuclear news aggregation

service provides latest news and information on nuclear issues - the JRC's web crawlers scan hundreds of newspapers every few minutes.
NUCLEONICA's Conference Calendar can be used to enter information on forthcoming events, meetings, conferences etc. The user can decide if he wishes to share this information with other users. In this way a user-generated calendar of events is generated. Alternatively, the user can decide to keep the information in his personal diary.

6. Preservation of Nuclear Knowledge: Web-based Fuel Cycle Calculations with webKORIGEN

WebKORIGEN is a web-based user-friendly version of the KORIGEN code. KORIGEN, developed in the Karlsruhe Research Centre, constitutes a standalone package supporting the fuel depletion, reprocessing, and decay calculations. KORIGEN, originating from the ORNL ORIGEN code, is used in the German nuclear industry and by German licensing authorities for application to German light-water reactors. It enables reliable assessments of decay energy release from actinides, fission products and activated impurities in irradiated fuel and is routinely applied for purposes related to the safe handling, reprocessing and storage of spent fuel.

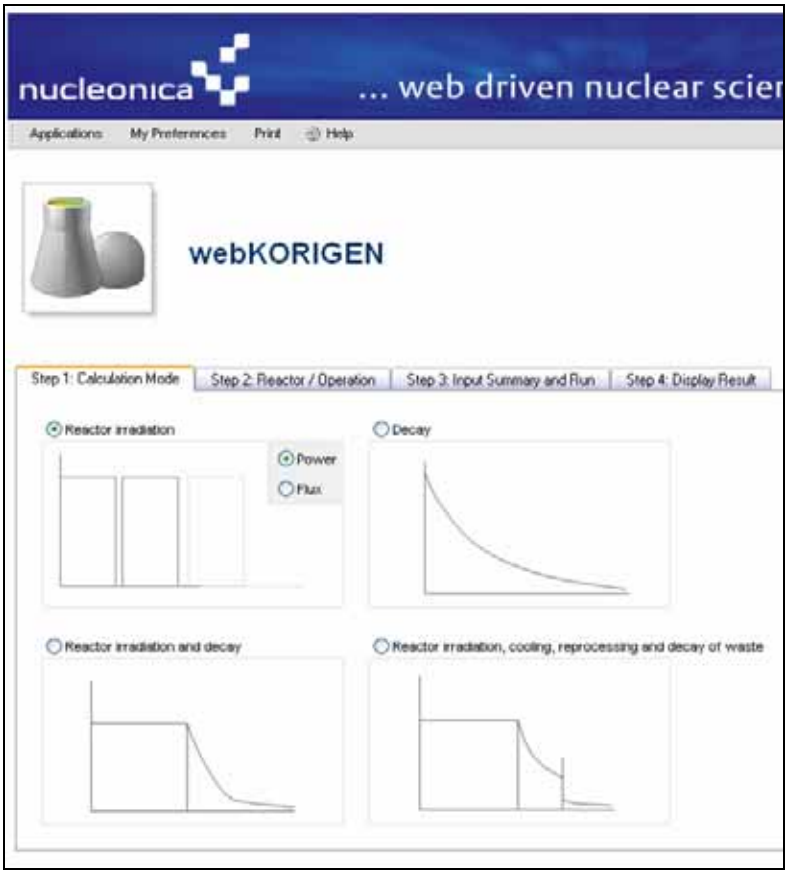

Fig 3. The webKORIGEN interface for fuel cycle calculations in NUCLEONICA.

By using webKORIGEN, advanced performance-based assessments of selected integral nuclear fuel cycle (NFC) characteristics can be done. It is applicable to both industrially practised, current and future advanced NFCs implementing the partitioning and transmutation (P&T) processes. The fuel cycle options in webKORIGEN cover "once-through " uranium-oxide NFC and "conventional reprocessing" NFC, the latter based on plutonium separation and single recycling in the form of uranium-plutonium mixed-oxide fuel. The webKORIGEN depletion engine uses facility data for thermal and fast systems; among them

the Pressurized and Boiling Water Reactors, and the European Fast Reactor. WebKORIGEN belongs to the isotopic summation codes which explicitly calculate, for a large set of isotopes, time dependent mass concentrations, radioactivities, decay heat and radiotoxicities of the nuclear material irradiated in a reactor core. Thus for the depletion calculations the complete nuclear databases must be supplied and managed. These data, prepared in advance, are transferred on demand to webKORIGEN from linked dedicated libraries. Their accuracy, benchmarked with experiments, warrants the reliable performance of the code.

7. Conclusions

NUCLEONICA is a web portal specifically dedicated to education, training and knowledge management in the nuclear sciences. In addition to providing internationally evaluated nuclear data, the portal provides access to a variety of nuclear science applications ranging from dosimetry and shielding to detailed fuel cycle calculations. NUCLEONICA's networking features allow users to stay in contact with colleagues, meet scientists with similar interests and build up an international contact list. The NucleonicaWiki provides a powerful content management system for online Help, ReadingRoom (for articles, and presentations), weblinks, element information, "ask an expert", etc., and in addition for information on the Karlsuhe Nuclide Chart [12].
With NUCLEONICA, there is no need to install software - all data and software is server-based. The development team takes care of maintaining the datasets and software and can add user options in response to customer demand. Further Information on registration [13] is available on the NucleonicaWiki.

8. References

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AN INTERACTIVE WEB ACCESSIBLE GAMMA-SPECTRUM SIMULATOR

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ABSTRACT

A versatile γ-spectrum simulation tool has been developed to allow the generation of accurate γ-spectra for a wide range of NaI and HPGe detectors and for any mixture of γ-emitting radionuclides. The simulator provides full interactive control of a virtual γ-spectrometer for modeling various geometries with shielded and unshielded sources. The output consists of an interactive graph, containing cumulative and nuclide specific spectral distributions. More detailed spectral information and a detection efficiency graph are available as advanced options. The simulator, which can be accessed through the NUCLEONICA nuclear science and data portal, is a powerful tool for providing basic and advanced training in various areas of nuclear science and applications.

1. Introduction

Nowadays the γ-spectrometry is used on a daily basis in different basic and applied fields of nuclear science and technology. A variety of instruments and measurement techniques, involving γ-spectrometry measurements, are employed routinely by nuclear and radio-chemists, health physicists, nuclear facility operators, radiation protection staff, safeguards inspectors, border police, customs and low-enforcement officers. Needs for education and training in these areas are high and, obviously, they will be increasing in the future as new challenges, such as strengthening nuclear safeguards and security, nuclear terrorism prevention and implementation of new standards in radiation safety and protection, arise. Contemporary web technologies coupled with advanced mathematical simulation can offer unique possibilities to address these growing demands by providing realistic visual interactive web-accessible teaching aids and tools. This paper reports on the first stage of the development of such a realistic web-based simulation tool, the Gamma Spectrum Generator, which can be accessed through the NUCLEONICA [1] nuclear science and data portal at www.nucleonica.net.

2. Basics of the simulation approach

The current implementation of a virtual measurement setup is based on a point-like γ-ray source located on the axis of a cylindrically symmetric NaI or High-Pure Ge (HPGe) crystal (the sensitive volume of a γ-spectrometer) and separated from it by a number of absorbing layers, as shown in Fig.1. The γ-spectrum for such measurement setups is constructed by summing appropriately normalized detector response profiles, generated for individual γ-rays emitted by a source.
The response profiles consist of peak and continuum components. The former includes the full energy peak (FEP), single and double escape peaks (SEP and DEP), X-ray escape peaks (XEP), and the 511 keV annihilation peak. The continuum component contains two contributions, both coming from Compton scattering events, which occur either inside a detector crystal or its surroundings. Although it is continuous in nature, the latter is often referred as a backscatter peak.

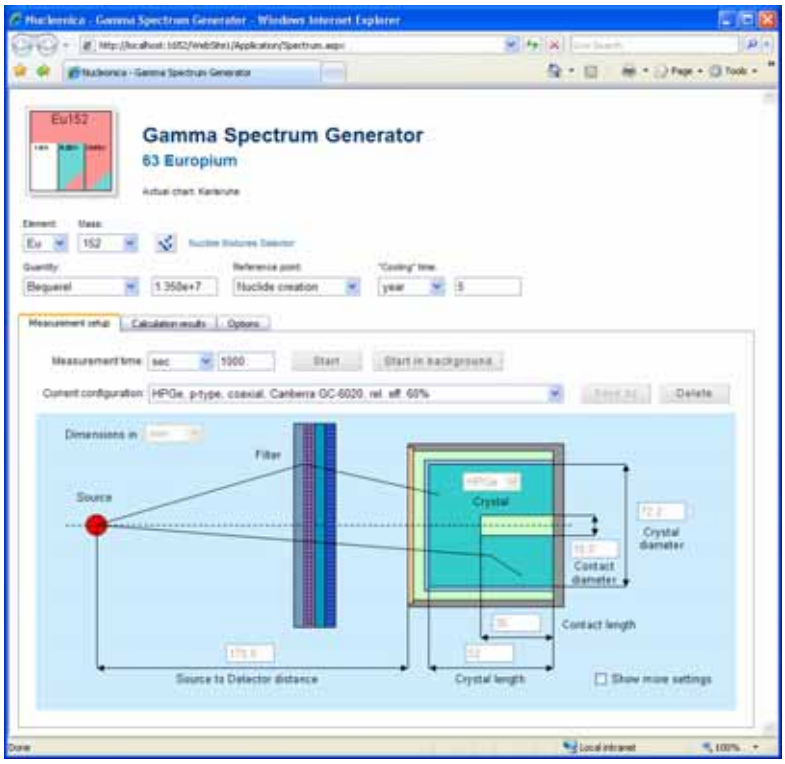


Fig 1. A screen capture of NUCLEONICA's Gamma Spectrum Generator web-page showing a tab with basic measurement geometry setup controls.

The relative contributions of the spectrum components are evaluated using an extensive detector response database, which has been created with help of a specially developed and validated Monte Carlo program. The database contains a large set of the peak-to-total and continuum-to-total efficiency ratios, and parameterized continuum shapes, calculated on grids of detector crystal dimensions, γ-ray energies and source-to-detector distances. In the course of modeling, a set of special interpolation techniques [2] is applied to calculate the efficiency ratios and continuum profiles for an arbitrary measurement setup and photon energy. Gaussian and Voigt distributions are used to model shapes of γ- and X-ray peaks, respectively. The peak widths represent actual energy resolution of a detector with additional contributions from Doppler broadening and natural line widths.
Once the relative response profile is constructed, it is converted to absolute values by performing normalization to the total detection efficiency. This efficiency is calculated by numerical integration over a detector crystal volume for the specified location of a source. The final response normalization is performed to account for the emission probability of particular γ-ray and actual number of decays of a respective nuclide, occurred during spectrum measurement. The latter is calculated based on the extended Bateman's analytical solution [3] of the system of differential equations governing radionuclide buildup and decay during source cooling and spectrum measurement time intervals.
Evaluated reference nuclear decay and photon attenuation data available in NUCLEONICA are used throughout spectrum modeling.

3. Features implemented

Fig.1 shows main features implemented in Gamma Spectrum Generator web-page. Using respective controls, an arbitrary individual nuclide or a pre-defined mixture of nuclides can be selected as a radiation source. A nuclide or a mixture of interest may be chosen also from NUCLEONICA's Nuclide Explorer or Nuclide Mixtures pages, which can be reached using corresponding links. Once a source nuclide is selected, the box at the top left of the page shows an image with its basic properties (decay modes, half-live, existing isomers) indicated. The nuclide's name to the right of the image provides a link to a part of the NUCLEONICA

Wiki, which describes in detail properties of the chemical element. The quantity (activity, mass or number of atoms) of a nuclide or a mixture can be specified either at the moment of its production/certification or at the spectrum measurement starting point of time. In the former case controls for specifying duration of a source cooling time interval become available.

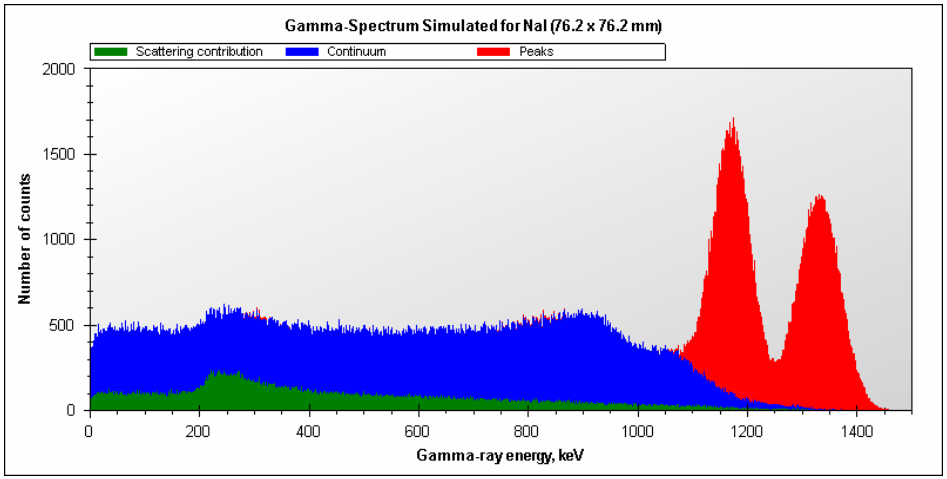
The spectrum measurement time and γ-spectrometer parameters can be specified on "Measurement setup" tab. Using the "Current configuration" dropdown list, one can choose a suitable γ-spectrometer from 6 pre-defined configurations, which include 2 coaxial HPGe detectors with 50% and 150% relative efficiency, low-energy (LEGe) and broad-energy (BEGe) HPGe detectors, and 2 scintillation detectors with standard ∅3″×3″ and ∅2″×1″ NaI crystals. The last entry ("Edit") in the drop-down list switches controls on the underlying measurement setup to the edit mode, whereby one can configure his own γ-spectrometer. The configurable parameters include the source-to-detector distance, as well as dimensions and materials of the detector construction elements, such as the detector crystal, crystal reflector, crystal packaging, crystal inactive layer, and the detector input window. All dimensions can be entered in "mm", "cm" or "inch" units. In addition to the crystal length and diameter, the dimensions of a cylindrical contact at the rear side of the crystal (a construction feature of conventional coaxial HPGe detectors) can be specified. Up to 6 additional absorbing filters made of Al, Cu, Fe, Pb, Sn, or polyethylene can be placed between source and detector, if one wants to reduce unwanted contribution to the simulated spectrum from the intense low-energy γ-radiation. The user can also add these filters to his virtual spectrometer configuration to simulate γ-spectra from containerized sources. Additional controls for specifying the detector energy resolution properties, number of spectrum channels and channel-to-energy conversion coefficient appear when "Show more settings" checkbox at the bottom right of the measurement setup drawing is selected. Once the user-specific γ-spectrometer is created, it can be saved in user's personal account in NUCLEONICA for future reference and use.

One can start calculations either in an on-line or background mode. In the latter case a notification will be sent via email and a respective alert will be raised in one's NUCLEONICA account, once the task has been completed. There are more settings on the "Options" tab, which provide additional control over the spectrum simulation. For instance, one can enable or disable decay calculations that will or will not allow contributions from decay products, being accumulated during source cooling and spectrum measurement time intervals. The backscatter peak simulation can be also switched on and off, and its contribution to the total detection efficiency can be adjusted using a special scaling factor.

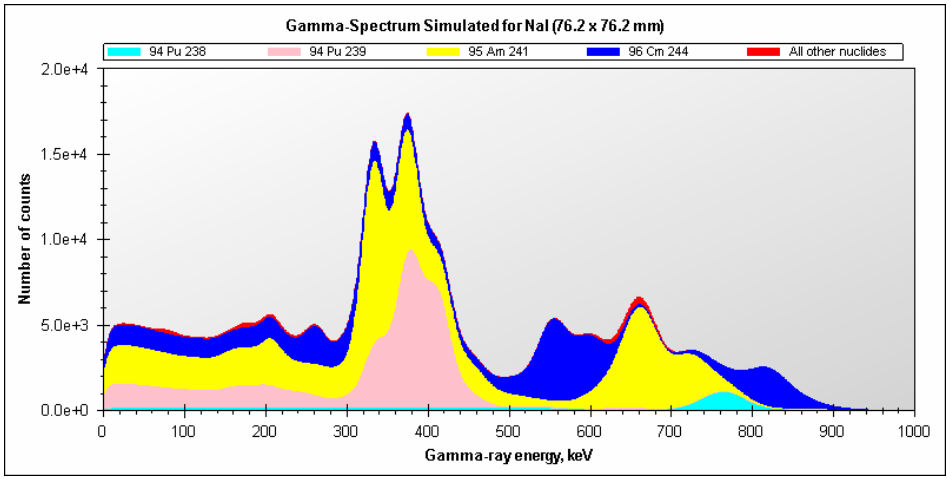
The standard output, which appears in "Calculation results" tab, consists of a stacked graph displaying cumulative and nuclide specific spectra, as well as peak, continuum and backscatter photon contributions to the full spectrum (see Fig.2). One can easily switch between types of spectral information presented on the graph, which include probability density functions for the detector input count rate at start or end of the measurement, as well as mean or statistical (Poisson) number of counts accumulated in spectrum channels. The graph is accompanied by brief numerical information on the total and nuclide specific count rates and number of spectrum counts. Additionally, a graph displaying total detection efficiency for the current spectrometer setup, as well as FEP, SEP, DEP and XEP efficiencies as functions of the incident photon energy can be activated. For both, spectrum and efficiency graphs, a set of controls are provided to tailor their appearance to one's needs and requirements and to download the final image in different graphics formats. A detailed report, containing the complete collection of spectral and efficiency numerical data, is generated also and can be downloaded as a text or Excel spreadsheet file.

4. Some examples

A number of graphs, demonstrating the capabilities of the Gamma Spectrum Generator, are shown in Fig.2. All graphs were created using the generator's tools and downloaded directly from its web-page.



(a)



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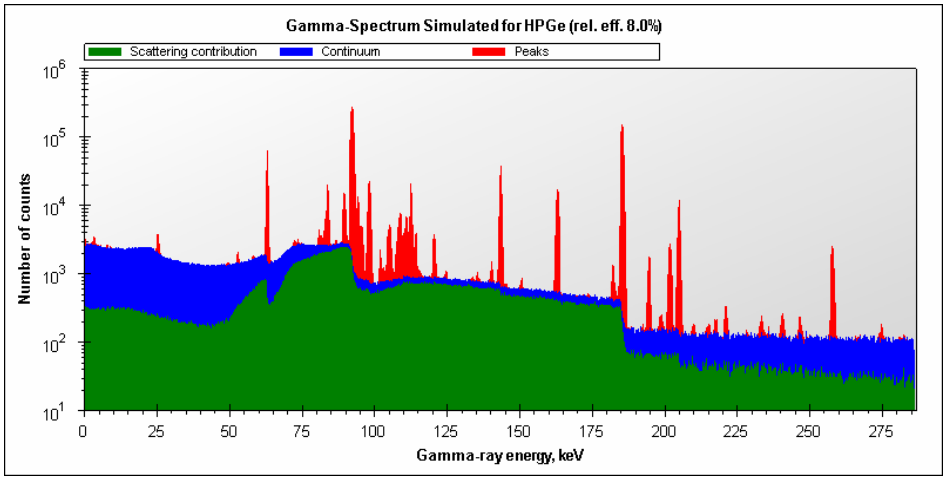

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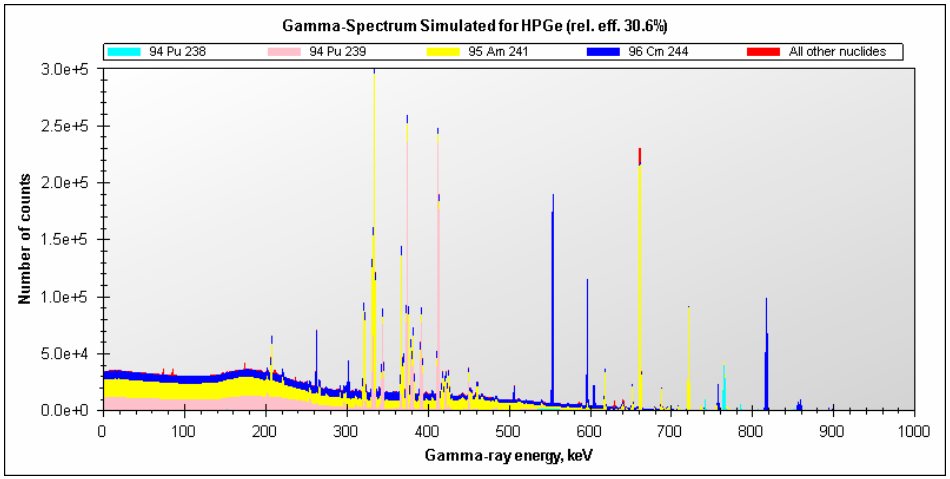

(d)

Fig 3. γ-spectra simulated for: (a) ^{60}Co 100 kBq source and NaI (∅3″×3″) detector, (b) 1 g natural U sample shielded with 0.5 mm Sn and LEGe (20 mm × 2800 mm^2) detector, (c) actinides in 1 kg PWR spent fuel shielded with 5 mm Pb and NaI (∅3″×3″) detector, and (d) actinides in 1 kg PWR spent fuel shielded with 5 mm Pb and BEGe (30% rel. eff.) detector.

Fig.2a shows γ-spectrum simulated for a 100 kBq ^{60}Co source and NaI (∅3″×3″) detector. The source is assumed to be positioned at 25 cm distance from the detector and measured for 1000 s. The graph demonstrates a powerful feature of the generator, which allows to visualize peak and continuum components of the spectrum. In addition, a backscatter peak contribution is shown as a separate continuum component in the graph.
The backscatter photon contribution looks more complicated in the γ-spectrum in Fig.2b. The spectrum was simulated for a 1 g U sample located at 2.5 cm distance from LEGe detector (crystal length 20 mm, active area 2800 mm^2) and shielded with 0.5 mm Sn filter. It was assumed that U had been separated from the ore 2 years before the measurement and had natural abundances of ^{234}U, ^{235}U and ^{238}U at the date of the separation. The spectrum includes contributions from all decay products, which have been accumulated since this date. To obtain better statistics of counts, the spectrum measurement time was 10^5 s.
Fig.2c and Fig.2d show low- and high-resolution γ-spectra for a 5.25 TBq source, which represents actinides extracted from a 1 kg sample of 6-year-aged PWR spent fuel. The isotopic composition of the fuel was calculated using NUCLEONICA's webKORIGEN [4], assuming 4.2% for the original enrichment and 50 GWd/t for the final burnup of the fuel. The low- and high-resolution spectra correspond to NaI (∅3″×3″) and BEGe (30% rel. eff.) detectors, respectively. In both cases the source was assumed to be shielded with a 5 mm Pb filter and located at 25 cm distance from the detectors. The measurement time is 1000 s. From the spectra shown one can see easily the advantages of the high-resolution γ-spectrometry when accurate characterization of the sample is required.

5. Future work

The capabilities of the Gamma Spectrum Generator are planned to be further extended to include simulation of the spectrum distortion effects (e.g. due to coincidence summing and energy resolution deterioration), which may appear in measurements involving elevated count rates and small source-to-detector distances. It is also foreseen to extent the detector response profile database to include $LaBr_3$ scintillators that, because of their much superior energy resolution, start to replace traditional NaI crystals in many applications. Inclusion of self-attenuation effects is another challenging task, which would allow more realistic simulation of γ-spectra from voluminous sources.

6. Conclusions

A versatile web-accessible γ-spectrum simulation tool has been developed to allow generation of accurate γ-spectra for a wide range of NaI and HPGe detectors and for any mixture of known γ-emitting radionuclides. The simulator is a useful visual teaching aid in providing basic and advanced training for members of nuclear and non-nuclear communities working in various areas of science and technology. The simulator tool is especially useful in training facilities, which have restrictions on the use of radioactive substances, or when sources of special interest (e.g. spent fuel, enriched U, weapon grade Pu or other highly radiotoxic materials) are not readily available.

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WEB-BASED DOSIMETRY AND SHIELDING CALCULATIONS IN NUCLEONICA

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ABSTRACT

The dosimetry and shielding module in Nucleonica allows the user to calculate gamma dose rates from point sources of either single nuclides or composite mixtures. The intuitive interface allows quick and accurate calculations. The present paper provides a detailed description of the module, in addition to discussing potential applications, particularly for education and training purposes.

1. Introduction

The new nuclear science web portal Nucleonica [1] has been developed at the Institute for Transuranium Elements. Nucleonica offers a suite of applications ranging from a powerful user-friendly Nuclide Explorer, which allows the user to navigate the nuclide chart and explore the properties of nuclides, to various computational and networking modules. One of the first modules developed was for dosimetry and shielding calculations for radioactive point sources and nuclide mixtures. The formalism for the dosimetry and shielding calculations is given in the Nucleonica wiki together with a detailed description [2] of the interaction of radiation with matter which provides the underlying physical basis.

2. The Dosimetry & Shielding Module

The dosimetry and shielding module allows the user to calculate gamma dose rates from point sources of either single nuclides or composite mixtures. It is possible to obtain the corresponding dose rate given a specific shield material and thickness. Alternatively, it is possible to calculate the material shielding thickness required to obtain a desired dose rate. More than 3000 nuclides and excited states with more than 53,000 gamma and x-rays are available in the Nucleonica database for dosimetry calculations, together with a choice of ten different materials for shielding purposes. The intuitive interface allows quick and accurate calculations and has been specifically designed to be suitable for use by professionals and students in nuclear science and technology.

2.1 Interface

The main interface, shown in Fig. 1 allows the users to select the nuclide, the source strength, the source/detector distance, the shield material and shield material thickness. In the example shown in Fig. 1, Co-60 ground state has been selected using the drop down menus. In the upper left hand corner, a graphic of the selected nuclide shows the half-life of the selected nuclide, 5.27 y, and information on the metastable state Co60m. The source strength can be set in different units, namely Activity (Bq), Activity (Ci), Mass (g) or number of atoms. The default value shown in Fig. 1 is 1 MBq. In addition, the user has the choice of 10 shield materials: lead, concrete (dry), tin, tungsten, uranium, water, aluminium, air (dry air at sea level) and tissue. The calculation is initiated by clicking in the Start button. The detailed results, shown in Fig. 2 in tabular form below the main interface, include the half-value layer (HVL) and the tenth value layer (TVL) thicknesses required to reduce the gamma

dose rate to 50% and 10% respectively of the initial value, and the specific gamma dose rate constant for the given nuclide.

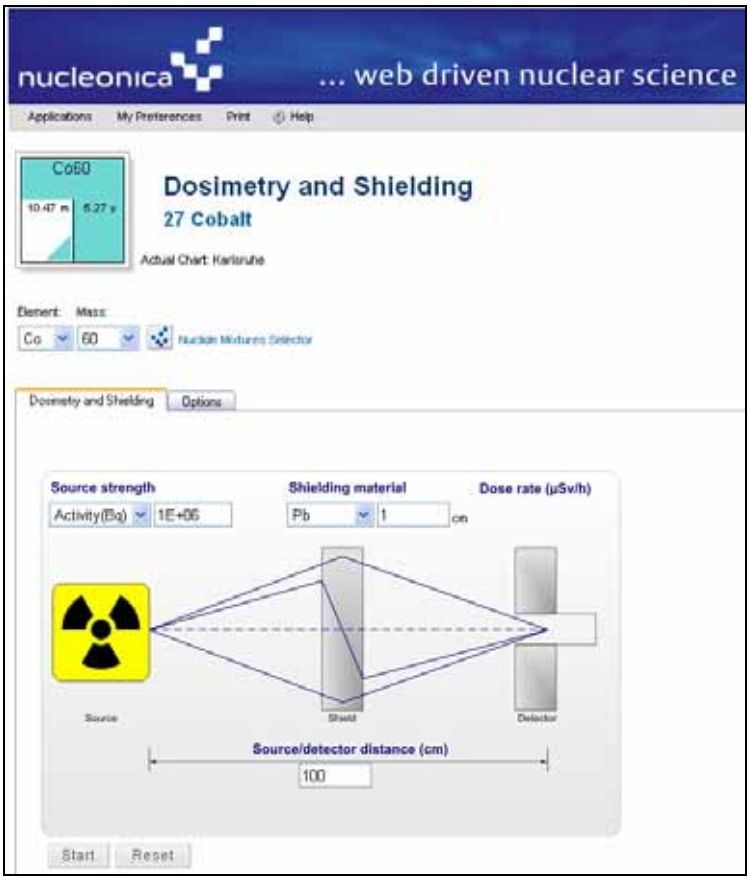

Fig 1. Dosimetry & shielding module interface.

Half-Value Shield Thickness(cm)	1.88E+00
Tenth-Value Shield Thickness(cm)	4.90E+00
Equivalent Dose Rate Constant Γ(mSv·m²/GBq/h)	3.37E-01
Gamma Dose Rate (µSv/h)	2.52E-01

Download ◉ Excel ○ CSV Separator: Semicolon (";") ☑ Use field qualifier (")

Number of lines (γ):	6	ΣE.P.(γ):	2.50E+06
Number of lines (X):	4	ΣE.P.(X):	8.35E-01
Number of lines (γ+X):	10	ΣE.P.(total):	2.50E+06

Download ◉ Excel ○ CSV Separator: Semicolon (";") ☑ Use field qualifier (")

Nuclide	Gamma Energy (MeV)	Emission Probability P (per disintegration)	Mass Attenuation Coefficient (shielding)(cm²/g)	Number of Mean Free Path(µd)	Build-up Factor	Mass Absorption Coefficient (tissue)(cm²/g)	Gamma Dose Rate(µSv/h)
27 Co 60	1.33E+00	1.00E+00	5.64E-02	6.40E-01	1.46E+00	2.89E-02	1.36E-01
27 Co 60	1.17E+00	9.99E-01	6.20E-02	7.04E-01	1.46E+00	2.98E-02	1.16E-01
27 Co 60	8.26E-01	7.60E-05	8.59E-02	9.75E-01	1.43E+00	3.16E-02	4.92E-06
27 Co 60	3.47E-01	7.50E-05	3.05E-01	3.46E+00	1.67E+00	3.21E-02	2.02E-07
27 Co 60	7.48E-03	6.44E-05	2.71E+02	3.07E+03	1	1.22E+01	0
27 Co 60	7.46E-03	3.27E-05	2.72E+02	3.09E+03	1	1.23E+01	0
27 Co 60	8.26E-03	1.31E-05	2.11E+02	2.40E+03	1	9.01E+00	0
27 Co 60	2.16E+00	1.20E-05	4.54E-02	5.15E-01	1.48E+00	2.52E-02	2.65E-06
27 Co 60	8.50E-04	1.49E-06	7.16E+03	8.12E+04	1	5.38E+03	0
27 Co 60	2.51E+00	2.00E-08	4.39E-02	4.99E-01	1.24E+00	2.40E-02	4.15E-09

Download ◉ Excel ○ CSV Separator: Semicolon (";") ☑ Use field qualifier (")

Fig 2. Detailed results for a 1 MBq Co-60 source.

This information is followed by the number of gamma and X-ray energies used in the calculation together with the quantity $\Sigma_i E_i \cdot P_i$ which is the sum of the energies multiplied by their emission probabilities. In the table in Fig. 2, the results include the contribution of each gamma-line or X-ray to the total dose rate, the mass absorption coefficients for tissue, the build-up factors, and the mass attenuation coefficients for the shield material (for refs. see [2]). The information can be re-arranged by clicking on the column headers. In the example shown in Fig. 2, clicking on the column header "Gamma Dose Rate (µSv/h)" re-arranges the table to show the main contributions to the gamma dose rate. In the case of Co-60 this is from the 1.33 and 1.17 MeV gamma lines. The information given in Fig. 2 can also be downloaded for further processing.

2.2 Basis of the Calculation

The dose rate is calculated using the point source kernel approach and is given by [3]:

$$\frac{dH(r)}{dt} = \frac{A}{4\pi r^2} \cdot \sum_i \left[E_i \cdot P_i \cdot \left(\frac{\mu}{\rho}\right)_i^{tissue} \cdot B_i \cdot \exp\left[-\left(\frac{\mu}{\rho}\right)_i^{shield} \cdot \rho d \right] \right]$$

where H(r) is the equivalent dose at distance r, A is the source activity and d is the shield thickness. The summation is over all lines i: E_i and P_i are the gamma energies and emission probabilities per disintegration, $(\mu/\rho)^{shield}$ is the mass attenuation coefficient in the shield material, $(\mu/\rho)^{tissue}$ is the mass absorption coefficient in tissue, and B_i is the dose build-up factor. In Figs 1 and 2, the calculated dose rate is 0.25 µSv/h at 1m with 1 cm Pb shielding.

2.3 Options

The Options window can be access from the appropriate tab in Fig. 1. There are two modes of operation. The user can obtain a dose rate with a given shield material and thickness. Alternatively, the thickness of shield material required to obtain a given dose rate can be calculated. The user can choose to include only gammas, X-rays, or both in the calculations. In addition, the threshold energy for contributions to the dose rate can be set by the user. The default value is 15 keV – photons with lower energy are absorbed by the outer layers of human tissue and do not contribute to the whole body dose.

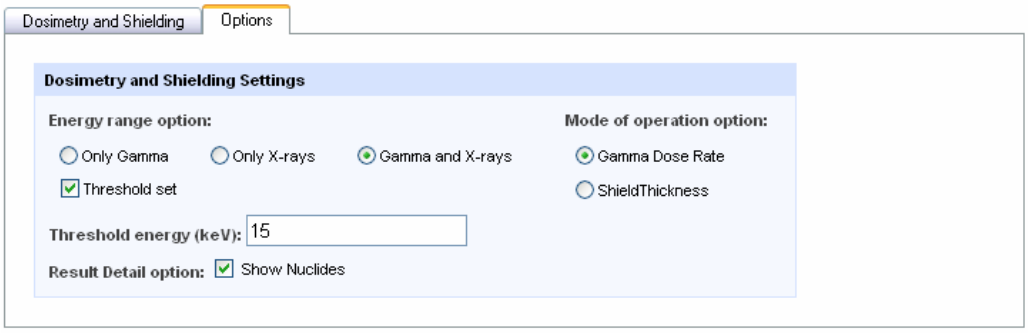

Fig 3. The Options window

3. Some Examples

3.1 Example: Occupational Exposure in Nuclear Medicine Departments

Tc-99m is a commonly used isotope in nuclear cardiology as a "tracer" for high image quality visualisation of organs. It is well suited to the role because it emits readily detectable 140 keV gamma rays, and has a short half-life of 6.01 hours. After approximately 10 half-lives, Tc-99m has almost completely decayed to its long-lived daughter Tc-99. The biological half-life of Tc-99, however, results in earlier removal from the body. A patient is injected with typically 30 mCi of Tc-99m. The treated patient must, therefore, be considered as an

unshielded source of radiation. During this time the radioactivity is present in the body, the medical staff - nurses, physicians and operators - will be exposed to radiation from the patient. It is thus interesting to estimate the dose rate received from a patient treated with 30 mCi of Tc-99m and to calculate how much shielding does a patient's body provides to protect his family and the medical staff. For this study we consider that the radioactivity is concentrated in the middle of the body (studies have shown, for example, that the technetium has tendency to concentrate in the kidneys) as a point source and shielded below 1 cm of human tissue. Calculations can then be performed with the dosimetry and shielding module of Nucleonica. The resulting gamma dose rate is 16.5 µSv/h, 65.9 µSv/h and 1.65×10^5 µSv/h at distances from the patient of 1 meter, 50 cm and 1 cm respectively. These figures are comparable with previous medical studies, see ref. [4]. If one considers that a typical procedure lasts for about 40 min, the exposure due to the patient requires the medical staff to be protected. The use of lead apron is compulsory for medical nuclear operators. From the dosimetry & shielding module, the dose rate behind a 0.5 mm lead apron at 1 m distance from the patient is reduced from 16.5 to 8 µSv/h.

3.2 Example 2: Handling of Spent Fuel in a "Hot-Cell"

The aim of this example is to demonstrate a shielding calculation with a mixture of nuclides, and to show the module working in the “shield thickness” mode. A "Hot-Cell" provides facilities for performing operations on highly radioactive material with minimal radiation exposure to the personnel involved. Most hot cells are designed to accept fuel rods for post irradiation investigations. To protect the user against gamma radiation, the different cells are shielded with lead bricks and can be operated through a lead glass window.

For this study we create a nuclide mixture, using the mixture option in Nucleonica, based on the main contributors to the gamma heat calculated using a webKORIGEN calculation of a spent fuel rod 4.2% enriched from a standard PWR reactor (50GWd/t) and after 6 years of cooling. The total mass of the 20 most important contributors to the total activity is 3.4 g per kg of spent fuel. The maximum mass load of spend fuel introduced into the hot cell is typically about 500g.

Fig 4. Results of a webKORIGEN calculation for the most important contributors to the gamma heat from spent fuel.

German regulations give a limit for occupationally exposed workers (category A) of 20 mSv/year assuming 2000 working hours (i.e. 2000 h of exposure). This leads to an hourly dose rate of 10 µSv/h for a regular worker working. The limit for occupationally exposed workers (category B) is 6 mSv/year assuming 2000 working hours (2000 h of exposure) hence equivalent to 3 µSv/h. We can then use the dosimetry and shielding module and using the "shield thickness" mode calculate the thickness of lead required to obtain 3 µSv/h at 1 m of distance for 1.7 g of the calculated mixture obtained with webKORIGEN. The calculation gives a lead thickness of 14.8 cm. In most of the existing hot cells, reinforced concrete walls provide the main shielding used for construction. The module has dry concrete as a shield option. This can then be used as an approximation for the concrete walls. The calculation gives a required thickness of 92.8 cm of concrete, as shown in Fig. 5. Typically, hot-cells have wall thickness of approximately 1 m of reinforced concrete and 1 m thick lead glass windows.

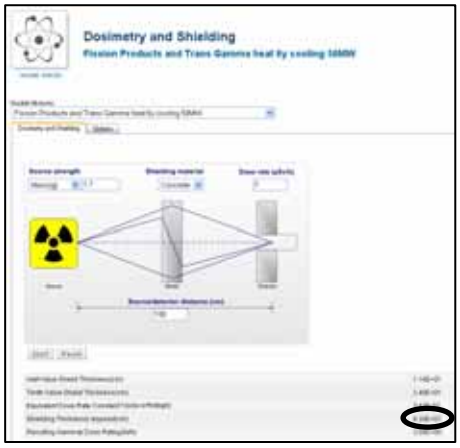

Fig 5. Calculation for the concrete shielding requirement for 1.7 g of the main transuranics elements and fission products, corresponding to 500g spent fuel.

4. Future developments

The Dosimetry & Shielding module in Nucleonica is under continuous development driven in particular by user demand. Future upgrades will include additional shielding materials, multilayer shielding options, and volumetric source dosimetry based on Monte Carlo calculations.

5. Conclusion

The dosimetry and shielding module in Nucleonica is a versatile tool for quick and accurate dosimetry and shielding calculations. It allows the user to calculate gamma dose rates from point sources of single nuclide and mixtures, through a choice of 10 different shield materials. Over 3000 nuclides with more than 53000 gamma lines are available in the database. The examples described provide an overview of the features available and the flexibility of the module for education and training purposes in nuclear science.

6. References

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http://content.onlinejacc.org/cgi/reprint/31/4/892

RANGE AND STOPPING POWER CALCULATIONS IN NUCLEONICA

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ABSTRACT

In the interaction between charged particles and matter, the stopping power or the average energy loss per unit path length plays an important role in many fields. Because of the great interest in this phenomenon, a web-based application has been developed in the Nucleonica portal to calculate the range and stopping power of electrons, positrons, protons, alphas, muons and heavy ions in a variety of different targets. The target materials can be selected from a variety of pre-defined elements and compounds. Alternatively, user-defined compounds can be created and stored for later use. The present paper provides a detailed description the range and stopping power calculations in Nucleonica. Agreement between the results and other well-known computer codes and experimental results shows that the module gives very reliable results. The application is suitable for professional use and for education and training purposes by educators and students in nuclear science.

1. Introduction

Stopping power, i.e. energy loss of energetic particles per unit length in matter, has been studied experimentally and theoretically since the beginning of the 20th century because of its wide application area, such as ion implantation, fundamental particle physics, nuclear physics, radiation damage, radiology, structure analysis of solid target by Rutherford backscattering spectroscopy, and plasma-first wall interaction in a nuclear-fusion reactor. Stopping power can be considered in two parts: first is the interaction of incident particle with target electrons (called electronic stopping power), and second is the interaction with target nuclei (called nuclear stopping power).

The first (classical) calculation of the energy loss of energetic particles was made by Bohr [1], while the first quantum mechanical treatment was done by Bethe [2]. This latter theory of stopping power is particularly accurate when the projectile's velocity is sufficiently high. Another important quantity is the range of the charged particle in matter. The range is defined as the mean path length of the particle in the target matter before coming to rest. Generally, analytic transport theory and Monte Carlo calculations are used for the range calculations.

Because of its importance, we have developed a web-based application for Range and Stopping Power (R&SP) calculations. One can easily calculate Range and Stopping Power for many types of projectile in various targets through the user-friendly interface in NUCLEONICA [3]. Full documentation of this module is given in the Nucleonica Wiki [4].

2. Projectile-Target Compositions

The user interface of the R&SP module is shown in Fig. 1. All pre-defined parts of module can be selected through the appropriate combo boxes in the main menu. Electrons, positrons, alphas, protons, muons, and ions with atom numbers from 1 to 92 can be selected from the "projectile" combo box shown in Fig. 1.

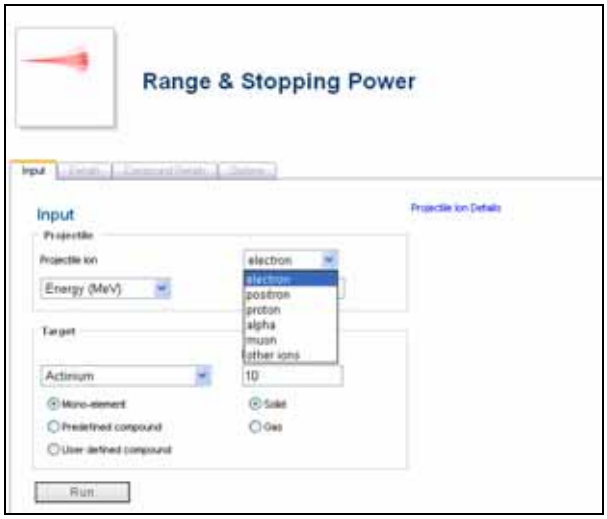


Fig 1. The RANGE module interface showing the types of projectiles available.

If the user selects "other ions", two new combo boxes appear. The first allows the user to choose an element from Z=1 to 92 and second allows selection of the isotopes. There are some limitations with regard to setting the energy of projectile. The module does not calculate stopping power and range if the projectile's energy is less than 10 keV or more than 1GeV for electrons and positrons, and less than 1 MeV or more than 1GeV for muons, and less than 1 keV or more than 2 GeV for alphas, protons and other ions.

For targets, the user can choose predefined mono-element from Z=1 to 92, predefined compounds, or user defined compounds. Pre-defined mono elements and compounds can be selected by using the corresponding radio buttons and combo box. Moreover, the target densities are taken form the Nucleonica database. By selecting the corresponding radio button, gas or solid state atomic density of the target is taken from the database. These values can, however, be changed in the density TextBox in main menu.

Users can create their own compounds by clicking the appropriate radio button and then "Compound Details" menu. In the compound details menu, one can add elements and their corresponding stoichiometry. User defined compounds can be given a name and saved for later use (Fig.2).

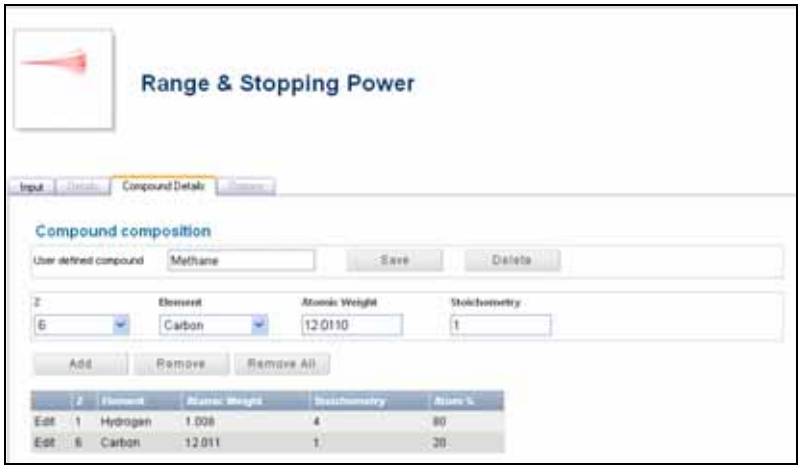


Fig 2. Interface for the creation of user-defined compounds.

Once the projectile and target have been selected/created, the calculations can be initiated by clicking the "Run" button. The results are then shown at the bottom of the page (see Fig.3).

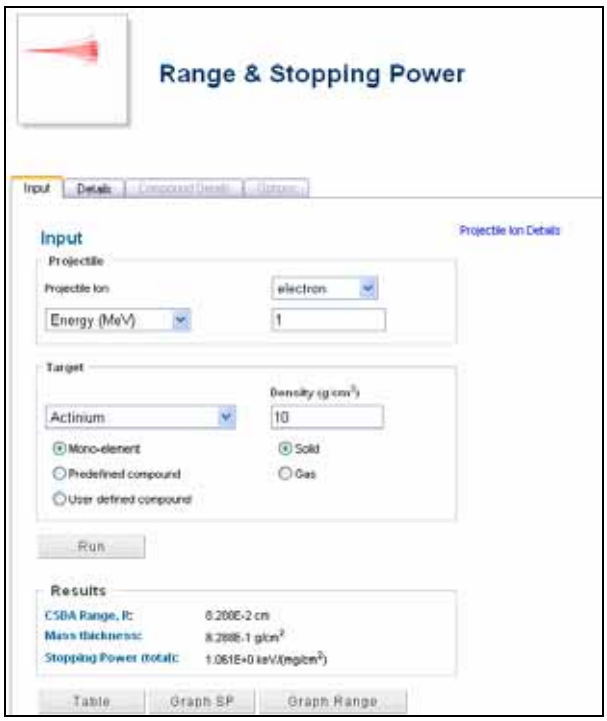


Fig 3. Main page of the Range module showing the input and summary results.

In addition to the summary results shown in Fig. 3 for a particular energy, the Range module creates a table of results for a wide energy range. This Table (button is shown at the bottom of Fig.3) contains projectile energy, electronic and nuclear stopping powers, the range, and the longitudinal and lateral straggling. Additional information is given in the results "Details" shown in Fig. 3. User can also see the graph of stopping power (Graph SP) and range (Graph Range) for the calculation. More details of the Range module can be found in Nucleonica Wiki [4].

3. Calculation Method and Theories Behind Range Module

The Range module uses different calculation methods depending on the type of the projectile. Mainly the SRIM [5] "engine" is used for heavy ions as well as alphas and protons. SRIM is a well known computer program developed by J.F. Ziegler and Biersack for the calculation of stopping power and range. This program includes many different methods including fitting to the experimental results. A detailed description of the calculation method can be found in *The Stopping and Ranges of Ions in Solids* [6].

In addition, we have used our codes for the calculations for electron, positron and muon projectiles. These calculations depend on previously developed and published methods. For electrons and positrons our codes are based on the work of H. Gümüş et al. [7,8]. Because the positron has the same mass and a charge opposite that of the electron, the structure of a positron track in matter is frequently assumed to be similar to that of an electron, so stopping power is calculated in a similar way to that of the electron. The Stopping Power calculation for electrons (or positrons) which are traversing through matter is similar to that of heavy charged particles. The interaction of incident particles with target electrons can be calculated from Bethe's theory, and this gives rise to the "Collisional Stopping Power". The interaction between incident particles (electrons or positrons) and target nucleus results in Bremsstrahlung, and this gives rise to the "Radiative Stopping Power". The collisional stopping power of matter is calculated by considering the effective charge approximation. When charged particles are accelerated or decelerated, they radiate and the energy of this

radiation can be any value from 0 to the energy of incident particles. This is the source of the radiative stopping power or Bremsstrahlung. This is more important especially for fast electrons (or positrons), since the mass of electron is much lower than that of nucleus it is accelerated more rapidly when it is in the coulomb field of nucleus. The strength of Bremsstrahlung depends on the target's atomic number (Z), and it is proportional to Z^2 and also proportional to incident energies. On the other hand, the collisional stopping power is proportional to Z. So, the ratio of the radiative stopping power to the collisional stopping power is approximately given by

$$\frac{S_{rad}}{S_{coll}} = \frac{ZE}{800} \qquad (1)$$

at high energies (more than 10 MeV), and E is the energy of the incident electrons in units of MeV. At high energies, this ratio can be used to calculate the radiative stopping power. The RANGE module uses this ratio to calculate radiative stopping power.

The muon is an elementary particle whose charge (-1 e) and spin (1/2) are equal to that of the electron. It is sometimes regarded as a "heavy" electron, because its mass is 207 times the electron mass and its interactions with matter are very similar to those of electrons. Muon interactions with matter differ significantly from electron interactions purely as a result of its much greater mass. For example the stopping power for electrons, particularly in the high energy regime, is dominated by the bremsstrahlung process, which is not the case for muons unless the energies are in the multi-GeV range. On the other hand, in this multi-GeV regime, radiative processes are more pronounced than for other heavy charged particles and ions. The Range module uses Bethe-Bloch equation for muons [9] for the calculation of stopping power.

Most of the transport calculations and Monte Carlo simulations for the calculation of Range are based on the so-called **C**ontinuous **S**lowing **D**own **A**pproximation (CSDA). In this approximation, it is assumed that the particle loses its energy in a continuous way and at a rate equal to the stopping power. Since the stopping power is the energy loss of projectile per unit path, CSDA range (or Bethe range) is calculated by

$$R(E) = \int_{E_{abs}}^{E} \frac{dE'}{S(E')}$$

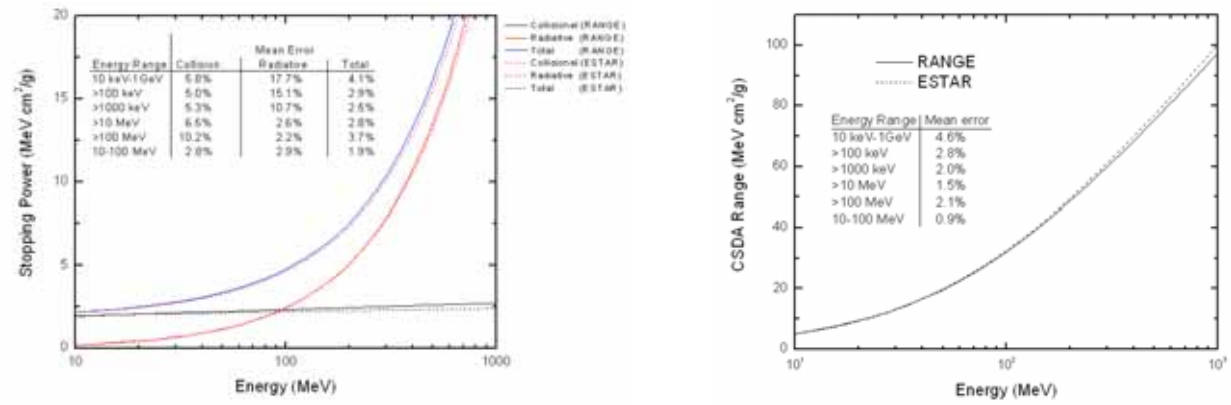
where E_{abs} is the energy where particle is effectively absorbed. The CSDA range is the path length travelled by the particle and since energy-loss fluctuations are not considered, the CSDA range is always higher than projected range (R_p) which is the distance between the point where particle enters the stopping medium and the point where particle is absorbed (or comes to rest). It becomes important when the projectile's energy is low enough. For electrons, positrons and muons, the Range module uses this approximation to calculate the range of the projectile in the matter.

4. Accuracy of the Range Module

To determine the accuracy of the Range module results, we have compared our results with various results in the literature. For electrons, protons and alphas in gas, solid and liquid phases for mono element and compound targets, we compared our results with the results obtained from the STAR program groups [10]. STAR program groups include three different stopping power and range calculation programs: ESTAR for electrons, PSTAR for protons and ASTAR for alphas. These programs were developed at the NIST. For positrons, we compared our results with the results given in ICRU 37 report [11]. For muons, we compared our results with the results given in Ref. [9]. The Range module uses SRIM for heavy particles with a known accuracy of less than 5%.

Test results show that agreements are less than 5% for protons and alphas, less than 10% for electrons and positrons, and less than 7% for muons. These results show the mean error and are for the total stopping powers and the CSDA Ranges.

For electrons and positrons, agreement is better than these results for collisional stopping power, however, for radiative stopping power mean error is higher because we use the simple ratio (Equation 1) to calculate the radiative stopping power.
For muons, the Range module uses the formulation which is indicated at the work of Groom et al. [9]. Because we calculate the stopping power at the energies below 1 GeV, we have calculated only collisional stopping power. However, the radiative stopping becomes important at high energies, so one must calculate also radiative stopping power. On the other hand, radiative stopping power is important above 100 GeV in almost all matter. This shows that our calculation can be also used at the energies above 1 GeV for muons.
Below, we give the graphs of the results of Range module for electrons in water as an example. The graphs include mean errors in Range module. Results for other projectiles and targets are given in the Nucleonica wiki [4].



(a) (b)

Fig 4. Range module results for electrons in water (liquid):
(a) the stopping power of water (liquid) (b) the range of electrons

5. Conclusions

The Range module in Nucleonica provides a user-friendly interface for quick and accurate calculations on the range and stopping powers of charged particles - electrons, positrons, protons, alphas, muons and heavy ions - in matter. Target materials include the natural elements, pre-defined and user-defined compounds. In addition, the user can also select the energy and stopping power units, etc. Range and stopping power results can be displayed in high quality graphs. The Range module can be used in the Nucleonica scripting language [12]. A detailed description of the Range module and the underlying theory is given in online Help in the NucleonicaWiki.

6. References

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NUCLEONICA – SOFTWARE DESIGN PATTERNS

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ABSTRACT

NUCLEONICA is the latest development in a family of information systems for the nuclear science community. Throughout this contribution some aspects of the internal structure of NUCLEONICA are described, in order to show the flexibility of the software architecture. In a typical 3-tier architecture it combines efficient databases with modern rich internet presentation techniques and a modular structure. Based on the Microsoft .NET framework it is well-suited to provide the ease of use today's computer users have come to expect. It is shown how web server, webservices, application libraries and the database repository are smoothly integrating with third party applications like MediaWiki that is used as a general help facility and as an interactive Q&A discussion forum.

1. Introduction

The evolution from the first predecessor through to NUCLEONICA reflects the software technical paradigm change from fat clients to a modern web application using latest Web 2.0 technology. NUCLEONICA's modular structure with the idea of *Software as a Service* in mind is well suited for integrating newly developed application modules such as the radiological dispersion module as well as well-known legacy codes such as KORIGEN [1] for nuclide depletion calculations in nuclear reactors. It was even possible to integrate an open-source framework like Mediawiki [2], being built on Apache, PHP and a mySQL database. Despite totally different code bases and database requirements a common single-sign-on for all applications could be realized.

The idea of providing an electronic knowledge base of physical nuclide data has a long history. There are two predecessor applications of NUCLEONICA each using a unique software technical approach – due to the technical possibilities and habits existing at the time, Nuclides 2000 [3] was a fat client Visual Basic application that installed on Windows PC's and was distributed on CD-ROM. It consisted of a database of nuclear data (Microsoft Access) and several applications, e.g. Nuclide Explorer (with far less functionality than in NUCLEONICA) and a decay engine. In that approach, updates weren't easily possible (new CD-ROMs had to be produced) and the platform was restricted to Windows based PCs. All algorithms were frozen to the scientific state when the CD-ROM was produced.

The next step towards web technology came with Nuclides.net in 2003 [4]. Still produced on CD-ROM with similar a design approach as that of Nuclides 2000, it shifted the applications part such as Decay Engine to a web application server at ITU in Karlsruhe, thus providing the possibility to keep step with the improving scientific models.

NUCLEONICA [5] now broke completely with the CD-ROM based approach through being accessible completely from the World Wide Web. Since there is no need to install software,, the applications open up also to Mac and UNIX users. The database information is always up to date and there's no longer need to support users with installation problems or to distribute

updates in case of program flaws. A major challenge however was the need to provide the necessary performance, because all concurrent users share the same central systems.

2. Modular architecture based on .NET

NUCLEONICA consists of four layers. The website itself is an ASP.NET 2.0 web application. It uses an SQL Server 2005 database, several DLLs (green) and services (red) that run on the same machine.

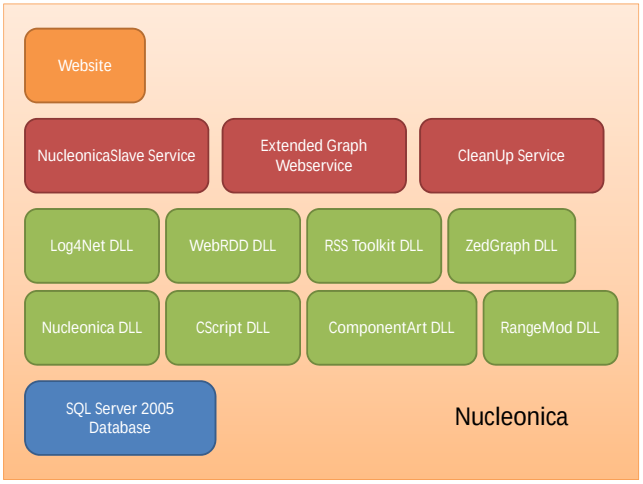

Fig. 1: NUCLEONICA Modular Architecture

Website	The ASP.NET pages the NUCLEONICA website consists of.
NucleonicaSlave	Long running asynchronous background executions
Extended Graph Webservice	Customizable generation of graphs, wraps ZedGraph.DLL
CleanUp Service	Housekeeping of temporary files
Log4Net DLL	Library for writing to the Windows event log (Error Handling)
WebRDD DLL	Library for computations in the RDD module
RSS Toolkit DLL	Library for RSS syndication
ZedGraph DLL	Library for graph generation (e.g. common graphics control)
Nucleonica DLL	Library for computations in most application pages. Common functionality like database access and collection types.
CScript DLL	Library for the NUCLEONICA Scripting Language components
ComponentArt DLL	3rd party library with enhanced user interface controls
RangeMod DLL	Library for Range & Stopping Power application
SQL Server 2005	Database server

Tab 1: NUCLEONICA modules and functionalities

The NUCLEONICA website shares a common look and feel on almost every web page. This is implemented via separate files, such as for a header and footer. Master pages are flexible page-templates allowing to "skin" and control the layout of the entire website by modifying a single template. This "visual inheritance" reduces maintenance and the overall complexity of the entire website.

NUCLEONICA uses a set of third party AJAX controls by ComponentArt [6], a vendor specializing in the creation of user interface and data visualization software for Microsoft's .NET platform. AJAX (**A**synchronous **J**avaScript **a**nd **X**ML) is a way of including content in a web page in which JavaScript code in the web page fetches some data from a server and displays it without re-fetching the entire page. The data fetched is often in XML format.

The Microsoft .NET Framework uses a managed code programming model. It consists of two main components, the common language runtime (CLR) and the .NET Framework class

library. The evolution process from Nuclides 2000 to NUCLEONICA includes a variety of grown, highly complex, nuclear scientific class libraries and applications. These had to be made accessible for the fully web-based NUCLEONICA. The challenge of integrating libraries written in various programming languages into NUCLEONICA while ensuring the security, robustness and stability of the legacy code reinforced the decision for the .NET Framework. Another essential point was the cross-language compatibility of Microsoft .NET. A multitude of developers contribute to the steady evolving progress of NUCLEONICA, each of them using the programming environment best suited to his task.

3. Web 2.0 – a gimmick or a vision?

Web 2.0, far from being merely a buzz-word of modern information technology, comprises some highly interactive, individually tailorable design patterns that aim at providing an interlinked computing platform by making use of the internet not only as an information resource but also as a scientific networking platform. *"…Web 2.0 is of course a piece of jargon, nobody even knows what it means*". Tim O'Reilly, known as the founder of O'Reilly Media, coined the term Web 2.0 in 2004 encompassing a new generation of web based services – such as wikis, communication, social networking and collaborative tagging. Seeing the internet as a participation platform he understands Web 2.0 as a new way of collaborating, collecting, constructing and experiencing in the World Wide Web. The constantly emerging techniques and features of modern web applications range from content syndication to interactive rich user interfaces. The evolution from Nuclides.net to NUCLEONICA, a fully web based portal service, opened the chance to involve the user more into the application. The following approaches are realized in NUCLEONICA:

Feature / Technique♣	Example
Rich Internet Application	- Nuclide Selector - Nuclide Explorer - Alerting Service - NUCLEONICA Portal
Content Syndication and Collaboration	- NUCLEONICA [Wiki] - ITU Nuclear News - NUCLEONICA Hot Topics - Conference Calendar
Social Networking	- NUCLEONICA Community Portal

Tab. 2: Web 2.0 Features of NUCLEONICA

The main goal was to combine rich and user-friendly interfaces with the approach of a web based scientific application suite, as well as an embedded social network for nuclear science experts.

Rich Internet Application

The combination of AJAX driven controls, customizable services and user-friendly user interfaces grants a highly flexible browser-based application. One of the frequently used controls - the "Nuclide Selector" - offers an AJAX-based way of selecting the nuclides for further processing.

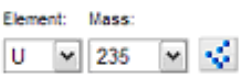

Fig 2: Nuclide Selector Control

In the first step the element is selected. This causes an AJAX *callback* to retrieve the mass numbers according to the element directly from the database. The selection of the desired mass number then initializes the *postback* to the server. Another usage of AJAX (on the server side) is the alerting control. This control notifies the logged in user about finished calculations, recent postings and messages. In these examples AJAX technology inconspicuously enhances the user interface without overloading and complicating it.

Content Syndication and Collaboration

The modern internet user not only acts as a consumer, but also as a contributor and/or producer. Therefore it was crucial to be aware of the relevance of user generated content (UGC). NUCLEONICA meets these requirements by offering the NUCLEONICA [Wiki] and the Conference Calendar. Users can exchange knowledge, information, support and events, resulting in a constantly growing mine of information – a benefit to all users. Beyond that NUCLEONICA provides a wide variety of nuclear news that can be accessed from the application or via the ITU Nuclear News Feed. The ITU nuclear news and the NUCLEONICA Hot Topics are distributed via Real Simple Syndication (RSS). RSS allows a user to subscribe to a page, not just to be linked to it. So, one is notified every time the pages changes or news are added. This makes NUCLEONICA a “live” application.

Social Networking

Another part of NUCLEONICA is the social network. Inside NUCLEONICA users can link and communicate with each other based on their common interests or scientific experiences. The network enables users to keep track of their contacts, groups and events.

4. Software as a service

Performance being an important issue with server based computing, it was necessary to have NUCLEONICA as modular as possible. The design goal bears in mind the possibility to distribute different parts of the application to different servers for load sharing and high availability issues.

The database (Microsoft SQL Server) runs totally independently and can easily be moved to another server without any code change due to the use of the .NET database interface.

Images such as graphs produced by the particular applications (Decay engine, Dosimetry and Shielding, etc.) have to be rendered in formats suitable to web browsers on one side. On the other hand it was also a design goal to support scientists with graphs of a quality appropriate for further uses such as in presentations or publications. For this purpose NUCLEONICA developers chose the freeware package ZedGraph [7] that was natively designed for Microsoft .NET and turned out to be extremely fast and produces graphs of convenient quality. It fits smoothly into the interfacing model of multi-instance applications without user interface that are typical running on a back-end server. As a consequence NUCLEONICA offers the ability to produce nice graphics not only as part of the nuclear applications but as a service for any type of data through the Extended Graph module. Moreover, in a next step this service will be offered as a webservice enabling scientists to make use of NUCLEONICA as part of their own local applications. As a proof of concept there’s already a plug-in for Microsoft Excel calling NUCLEONICA webservice for generating graphs (see Fig. 3). In future versions it is planned to provide more applications through webservice interfaces.

Long-running applications are tedious to the user especially in a web environment where one tends to consider everything that lasts longer than a few seconds as ”stuck“. The possibility of running complex computations asynchronously in the background and informing the user about results through email alerts underlines this service character of NUCLEONICA.

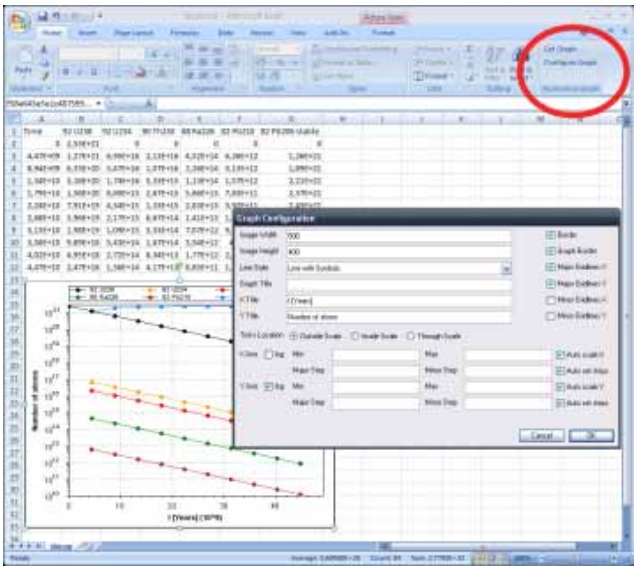

Fig. 3: Excel Plug-In for NUCLEONICA

5. Legacy Applications – don't re-invent the wheel!

Implementing NUCLEONICA as a web application was a major issue that should be made easier by re-using as much existing code as possible – both as far as system modules and libraries are concerned, and on the other hand as for nuclear and physical application modules.

As an example NUCLEONICA [Wiki] relies on the existing and well-proven technology of MediaWiki (itself built on the components of the freeware meta-package XAMPP Lite [8]). However extensions were implemented to realise for example the Single-Sign-On capability between NUCLEONICA (a .NET application) and MediaWiki, a PHP application. The NUCLEONICA user profits by not having to log in to the Wiki when coming from NUCLEONICA. Another example is the ZedGraph package (see above).

Scientific legacy code is built into the integrated nuclear software models. The webKorigen module for example is a piece of software developed over many decades. This module was integrated and combined with a modern web user interface.

Keeping in mind flexibility NUCLEONICA users are encouraged to integrate their own legacy algorithms. The integrated scripting language NUCLEONICA script, a dynamically parsed C like programming language offers access to all necessary database fields of the integrated nuclear knowledge base. It comprises all necessary language elements to write own code making use of the data and also of the integrated applications up to presenting textual and graphical results.

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