Precursors and decay events with EASY-II

Jean-Christophe Sublet and Michael Fleming

UK Atomic Energy Authority Culham Science Centre Abingdon OX14 3DB United Kingdom



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- FISPACT-II is a modern engineering prediction tool for activation-transmutation, depletion inventories, etc.
- The EASY-II system has been guided by TALYS n-TAL collaboration, which provides *complete* nuclear data libraries.
- FISPACT-II was designed to be a functional replacement for FISPACT-2007 but significant development has produced a substantially superior, more mature code
- a, g, d, p, n-Transport Activation Library: TENDL-2014 from the TENDL collaboration, but also ENDF/B, JENDL, JEFF
- Nuclear data processing done with (including cross-checks) NJOY (LANL), PREPRO (LLNL), and CALENDF (CEA-CCFE)







- All problems are multi-physics but usually decomposed into single physics ones
- The nuclear data, processing steps answers the needs of single physics codes (mainly reactor physics)
- Advanced simulation methods rely upon multi-physics codes with complex feedback
- This *requires* integrated, multifaceted processing steps able to deliver rich, interconnected type of nuclear data forms and correlated uncertainty
- This in turn requires the basic nuclear data to be complete but unique, robust, technological based with variancecovariance for every quantities across all energy ranges and decay schemes





 Set of stiff Ordinary Differential Equations to be solved



$$\frac{dN_i}{dt} = -N_i(\lambda_i + \sigma_i \varphi) + \sum_{j \neq i} N_j(\lambda_{ij} + \sigma_{ij} \varphi)$$

- Here λ_i and σ_i are respectively the total decay constant and cross-section for reactions on nuclide i
- σ_{ij} is the cross-section for reactions on nuclide j producing nuclide i, and for fission it is given by the product of the fission cross-section and the fission yield fractions, as for radionuclide production yield
- λ_{ii} is the constant for the decay of nuclide j to nuclide i





- LSODES, Livermore Solver for Ordinary Differential Equations with general sparse Jacobian matrices
 - Backward Differentiation Formula (BDF) methods (Gear's method) in stiff cases to advance the inventory
 - Adams methods (predictor-corrector) in non stiff case
 - makes error estimates and automatically adjusts its internal time-steps
 - Yale sparse matrix efficiently exploits the sparsity
 - ability to handle time-dependent matrix
 - no need for equilibrium approximation
 - handles short (1ns) time interval and high fluxes
- LSODES wrapped in portable Fortran 95 code
 - dynamic memory allocation
 - minor changes to Livermore code to ensure portability





- n-tendl-2014 (2013), multi temperature, 709 groups library; 2632 targets
 - ✓ full set of covariance
 - ✓ probability tables in the RRR and URR
 - ✓ xs, dpa, kerma, gas, radionuclide production
- JENDL-4.0u, ENDF/B-VII.1, JEFF-3.2, 709 groups libraries; circa 400 targets each
- g-tendl-2013, 162 groups xs library, 2629 targets
- p-tendl-2013, 162 groups xs library, 2629 targets
- d-tendl-2013, 162 groups xs library, 2629 targets
- a-tendl-2013, 162 groups xs library, 2629 targets





- Decay-2012, 3873 isotopes (23 decay modes; 7 single and 16 multi-particle ones)
- Ingestion and inhalation, clearance and transport indices libraries, 3873 isotopes
- ✓ JEFF-3.1.1 DD and FY, UKFY4.2 fission yields, GEF
- ✓ ENDF/B-VII.1 DD and FY (??)
- ✓ JENDL FPD/FPY (??) 2011
- ✓ EAF-2010 decay data: 2233 isotopes
- EAF-2010 ingestion and inhalation, clearance and transport indices libraries, 2233 isotopes
 - EAF's uncertainty files
- ✓ Decay-2015, at the assemblage level





FISPACT-II versus FISPACT-2007

	FISPACT-II	FISPACT-2007
Solver	Numerical - LSODES 2003	Numerical - EXTRA 1976
Incident particles	α, γ, d, p, n (5)	d, p, n (3)
EAF's libraries: EAF-2010, 2007, 2005, 2003	XS data (816 targets)Decay Data (2233 isotopes)	XS data (816 targets)Decay Data (2233 isotopes)
ENDF's libraries: TENDL-2014, ENDF/B-VII.1, JEFF-3.2, JENDL-4.0	✓ XS data (2632 targets)✓ Decay data (3873 isotopes)	×
Dpa, Kerma, Gas prod., radionuclide yields	✓	X (Gas production)
Uncertainty	✓ Variance-covariance	1 to 3 broad groups
Temperature	0, 294, 600, 900 K,30 KeV	294 K
Self-shielding	 Resolved and Unresolved Resonance Range 	\boldsymbol{x} infinitely dilute cross section
Energy range	1.0 10 ⁻⁵ eV – 200 MeV	1.0 10 ⁻⁵ eV - 55 MeV
Sensitivity	 Monte Carlo 	 sensitivity coefficient
Pathways	✓ multi steps	✓ single step
Thin, thick targets yields	\checkmark	×







Energy Control Carbon Faster

CCFE

CULHAM CENTRE FUSION ENERGY



> For all targets nuclei, incident particles and daughters

- Cross sections, angular distribution, emitted spectra
- Half life, masse, energy levels and schemes
- Decay schemes and energies
- Spontaneous, induced fission yields (single/cumulative)
- Resonance Integrals, Maxwellian, thermal
- Correlated uncertainty
- Spallation products
- Inhalation, ingestion hazards
- Transport, clearance indices





14 MeV neutrons are generated by a 2 mA deuteron beam impinging on a stationary tritium bearing titanium target; Fusion Neutron Source



FNS Neutron spectra, neutron fluence monitored by ²⁷Al(n, ☑)Na²⁴

Two experimental campaigns: 1996 and 2000; 74 materials

Z	Element	Form	\mathbf{Z}	Element	Form
9	Fluorine	CF_2	46	Palladium	Metallic Foil
11	Sodium	Na_2CO_3	47	Silver	Metallic Foil
12	Magnesium	MgO	48	Cadmium	Metallic Foil
13	Aluminium	Metallic Foil	49	Indium	Metallic Foil
14	Silicon	Metallic Powder	50	Tin	SnO_2
15	Phosphorus	P_3N_5	51	Antimony	Metallic Powder
16	Sulphur	Powder	52	Tellurium	${\rm TeO}_2$
17	Chlorine	$C_2H_2Cl_2$	53	Iodine	IC_6H_4OH
19	Potassium	K_2CO_3	55	Caesium	Cs_2O_3
20	Calcium	CaO	56	Barium	$BaCO_3$
21	Scandium	Sc_2O_3	57	Lanthanum	La_2O_3
22	Titanium	Metallic Foil	58	Cerium	CeO_2
23	Vanadium	Metallic Foil	59	Praseodymium	Pr_6O_{11}
24	Chromium	Metallic Powder	60	Neodymium	Nd_2O_3
25	Manganese	Metallic Powder	62	Samarium	Sm_2O_3
26	Iron	Metallic Foil	63	Europium	Eu_2O_3
Alloy	SS304	Metallic Foil	64	Gadolinium	$\mathrm{Gd}_2\mathrm{O}_3$
Alloy	SS316	Metallic Foil	65	Terbium	$\mathrm{Tb}_4\mathrm{O}_7$
27	Cobalt	Metallic Foil	66	Dysprosium	Dy_2O_3
Alloy	Inconel-600	Metallic Foil	67	Holmium	Ho_2O_3
28	Nickel	Metallic Foil	68	Erbium	$\mathrm{Er}_{2}\mathrm{O}_{3}$
Alloy	Nickel-chrome	Metallic Foil	69	Thulium	$\mathrm{Tm}_2\mathrm{O}_3$
29	Copper	Metallic Foil	70	Ytterbium	Yb_2O_3
30	Zinc	Metallic Foil	71	Lutetium	Lu_2O_3
31	Gallium	Ga_2O_3	72	Hafnium	Metallic Powder
32	Germanium	GeO_2	73	Tantalum	Metallic Foil
33	Arsenic	As_2O_3	74	Tungsten	Metallic Foil
34	Selenium	Metallic Powder	75	Rhenium	Metallic Powder
35	Bromine	BrC_6H_4COOH	76	Osmium	Metallic Powder
37	Rubidium	Rb_2CO_3	77	Iridium	Metallic Powder
38	Strontium	$SrCO_3$	78	Platinum	Metallic Foil
39	Yttrium	Y_2O_3	79	Gold	Metallic Foil
40	Zirconium	Metallic Foil	80	Mercury	HgO
41	Niobium	Metallic Foil	81	Thallium	$\mathrm{Tl}_{2}\mathrm{O}$
42	Molybdenum	Metallic Foil	82	Lead	Metallic Foil
44	Ruthenium	Metallic Powder	83	Bismuth	Metallic Powder
45	Rhodium	Metallic Powder			





Decay power: FNS JAERI Ni





Decay power: FNS JAERI Ni

Times	FNS EXP. 5 mins	TENDL-201	3	ENDF/B-VII.1	JEFF-3.2	JENDL-4.0
Min.	$\mu W/g$	$\mu W/g$	E/C	E/C	E/C	E/C
0.58	4.11E - 02 + /-6%	4.90E - 02 + / -22%	% 0.84	0.79	0.79	1.04
0.83	4.38E - 02 + / -6%	4.55E - 02 + / -22%	% 0.96	0.94	0.94	1.23
1.08	4.18E - 02 + /-6%	4.24E - 02 + / -21%	% 0.99	1.00	1.00	1.30
1.33	3.71E - 02 + / -6%	3.95E - 02 + / -21%	% 0.94	0.99	0.99	1.29
1.58	3.35E - 02 + / -6%	3.70E - 02 + / -21%	% 0.90	0.99	0.99	1.29
2.02	2.95E - 02 + /-6%	3.32E - 02 + / -20%	% 0.89	1.05	1.05	1.35
2.62	2.56E - 02 + / -6%	2.89E - 02 + / -20%	% 0.89	1.17	1.17	1.49
3.22	2.20E - 02 + /-7%	2.55E - 02 + / -20%	% 0.86	1.27	1.27	1.60
4.07	1.84E - 02 + /-7%	2.19E - 02 + / -21%	% 0.84	1.46	1.46	1.82
5.17	1.53E - 02 + / -7%	1.86E - 02 + / -22%	% 0.83	1.79	1.79	2.16
6.27	1.37E - 02 + / -7%	1.63E - 02 + / -23%	% 0.84	2.22	2.22	2.60
7.88	$1.19E{-}02 + /{-}7\%$	1.39E - 02 + / -24%	% 0.86	2.85	2.84	3.15
9.95	1.04E - 02 + / -8%	1.20E - 02 + / -24%	% 0.87	3.44	3.42	3.57
12.05	9.32E - 03 + / -8%	1.06E - 02 + / -24%	% 0.88	3.59	3.62	3.59
15.15	8.02E - 03 + / -7%	9.02E - 03 + / -24%	% 0.89	3.40	3.44	3.40
19.25	6.58E - 03 + / -7%	7.47E - 03 + / -24%	% 0.88	2.99	3.01	2.97
23.32	5.54E - 03 + / -7%	6.29E - 03 + / -23%	% 0.88	2.62	2.64	2.59
27.42	5.00E - 03 + / -7%	5.39E - 03 + / -22%	% 0.93	2.43	2.45	2.39
34.48	3.92E - 03 + / -8%	4.27E - 03 + / -22%	% 0.92	1.96	1.97	1.92
44.58	3.00E - 03 + / -8%	3.29E - 03 + / -23%	% 0.91	1.54	1.55	1.50
54.68	2.58E - 03 + / -8%	2.72E - 03 + / -24%	% 0.95) 1.35	1.36	1.31
Produ	ict Pathways	T_1	/2	Path $\%$	$\rm E/C~\Delta$	$\mathbf{E\%}$
Co62	Ni62(n,p)Cc	62 1.5	m	99.8	$0.90 6^{\circ}_{2}$	70
Co62m	Ni62(n,p)Co	62m 13.	$9\mathrm{m}$	100.0	$0.89 \ 7^{\circ}_{2}$	70





Decay power simulation with EASY-II



Simulation of SS316 irradiated in JAEA FNS m - metastable state(s) > 50%



Thermal ²³⁵U pulse generates a large inventory...

Each nuclide at $(x,y)=(t_{1/2},heat(t_{1/2}))$







Fission decay heat TAGS

Blue = Greenwood nuclides and WPEC SG 25 P1, P2, P3 are priority 1, 2, 3 nuclides with requested TAGS by subgroup 25











Fission pulse



- Selection of experiments usually used in validation of decay heat simulations
- Tobias is meta-analysis with exp from 1950s onward and modification of uncertainties to make fits

Author	Method	Nuclide	Irrad. (s)	Year
Yarnell, LANL	Calor.	²³⁵ U _{th} ²³⁹ Pu _{th} ²³³ U _{th}	2E4	1980
Dickens, ORNL	β,γ spec.	²³⁵ U _{th} ²³⁹ Pu _{th} ²⁴¹ Pu _{th}	1100.	1980
Baumung, KfK	Calor.	²³⁵ U _{th}	200	1981
Akiyama, YAYOI	β,γ spec.	$^{232}\text{Th}_{f}{}^{233}\text{U}_{f}{}^{235}\text{U}_{f}{}^{238}\text{U}_{f}{}^{239}\text{Pu}_{f}$	10300.	1982
Johansson, Uppsala	β,γ spec.	$^{235}U_{th,}$ $^{239}Pu_{th,}$ $^{238}U_{f}$	4120	1987
Schier, Lowell	β,γ spec.	²³⁵ U _{th} ²³⁸ U _f ²³⁹ Pu _{th}	<1	1997
Ohkawachi, YAYOI	β,γ spec.	²³⁵ U _f ²³⁷ Np _f	10300	2002
Tobias, CEGB	Meta-analysis	²³⁵ U _{th} ²³⁹ Pu _{th}	Pulse-1E5	1989





- Many fission decay heat experiments
- Different fission rate calculation methodologies
- Many nuclides: U235, U238, Pu239, Pu241, Th232, Np237
- Even more experimental fluxes ORNL 'thermal flux' ≠ Karlrushe 'thermal flux' ≠ LANL 'thermal flux' ≠ ...
- Even more irradiation schedules
 - Dickens 1 s irrad followed by 2 s waiting
 - Akiyama 10 s irrad followed by 6 s waiting
 - Karlrushe 200 s irrad followed by 15 s waiting
- 'Correction factors' <u>in experiments</u> to get burst function, fission rate normalisation, capture correction, epithermal contribution ...





 Each major library contains different sets of nuclides within decay sub-libraries, nFY and sFY

	ENDF/B-VII.1	JENDL-4.0	JEFF y
Decay data	3821	1285	3851
nFY	31	31	19
sFY	9	9	3

- nFY is function of incident neutron energy
 - Number of bins and placement chosen for simple applications
 - 3 nFY incident-energies will not be sufficient for more demanding analysis
- How do we obtain high-fidelity fine-grid nFY(E)??





- nFY in calculations are cumulative over 1ms pulse and thermal with mono-energetic 0.025 eV
- To focus on decays all nFY data here = JEFF3.1.1 nFY
- Calculations employ cumulative fission yields and are necessarily "contaminated" with the decay data used
- Small differences in decays of precursors can dramatically affect longer-term decays and heat
- Future work: will consider single fission event calculations to probe short timescale affects not possible in cumulative





Decay heat following a pulse of thermal neutrons



- All measurements shown. Under-estimation of gammas consistently
- Potential contamination from capture events and chain fissile decays!!





Better agreement with JENDL-4 and ENDF/B-VII for gamma







- Below are the dominant nuclides and their *gamma* heat contribution at 250s after pulse for ²⁴¹Pu_{th} in kW (normalised relative to ENDF/B-VII)
- The Tc nuclides are very different for JEFF-3.1.1dd!
- Non-negligible Cs140 and Sb133 increases for JENDL

Nuclide	ENDF/B-VII.1	Nuclide	JENDL-4.0	Nuclide	JEFF3.2/3.1.1
Tc105	21.4	Tc105	21.5	Sb133	16.9
Tc104	18.5	Sb133	21.2	1136	15.8
Sb133	16.7	Tc104	18.5	Sb132	14.3
1136	15.7	Cs140	16.7	Cs140	12.6
Sb132	14.3	1136	15.6	Sr93	11.0
Cs140	14.1	Sb132	14.9	Tc104	10.8
Sr93	10.8	Tc103	10.9	I	I
Pr148	10.4	Sr93	10.0	Tc105	7.9





- Below are the dominant nuclides and their *beta* heat contribution at 250s after pulse for ²⁴¹Pu_{th} in kW
- Sb133 beta same while gamma different for JENDL?
- Tc differences reflected in beta as well

Nuclide	ENDF/B-VII.1	Nuclide	JENDL-4.0	Nuclide	JEFF3.2/3.1.1
Xe137	25.9	Xe137	25.9	Xe137	25.9
Tc103	19.3	Rh108	19.1	Tc103	19.3
Rh108	18.5	Tc102	15.5	Rh108	18.6
Tc102	15.6	Cs139	15.1	Tc102	15.6
Cs139	15.2	Tc103	13.8	Tc105	15.4
I	I	I	I	Cs139	15.2
Tc105	9.0	Tc105	8.4	I	I
Tc104	5.3	Tc104	4.9	Tc104	9.2
Sb133	5.3	Sb133	5.1	Sb133	5.1





- 250s after pulse for ²⁴¹Pu_{th} in kW (x10 vs previous slides)
- Typically gamma +/- is reflected in beta -/+ but not all!
- Total should add, but sometimes do not
- The more nuclides considered, the more differences found!

Nuclide	ENDF Y	JENDL Y	JEFF Y	ENDF β	JENDL β	JEFF β
Pr148	104	72.5	104	75.1	98.9	79.1
Mo103	81.3	93.6	53.2	97.4	92.9	110
Rb90	84.8	70.5	74.1	71.1	64.9	62.5
Ce145	76.5	89.9	52.2	53.4	46.5	66.2
Tc103	48.8	109	48.9	193	138	193
Nb99m	30.5	82.4	31.2	66.0	56.8	68.0
La144	66.7	46.3	65.3	21.6	27.0	20.9
La143	20.1	12.5	21.0	58.2	71.2	59.0
Rb90m	18.4	28.8	34.3	5.32	12.5	9.93





Compared against Tobias U235 thermal pulse compilation







- Comparison with gamma heat shows clear discrepancies
- Nota bene No Lowell data in Tobias for short time-scales, Tobias overestimates below 100s
- <20 s Generally larger uncertainties with fewer measurements and more corrections/modifications





- C/C comparisons
- Below are the dominant nuclides and their *gamma* heat contribution at 4s after pulse for ²³⁵U_{th} in kW
- JENDL Rb94, Y96, Nb102m ↔ Nb102 (all have both)

Nuclide	ENDF/B-VII.1	Nuclide	JENDL-4.0	Nuclide	JEFF3.2/3.1.1
Rb92	80.4	Rb92	80.5	Rb92	65.4
Rb93	61.6	Rb93	55.4	Rb93	63.8
Zr99	46.5	Rb94	47.2	Nb102	60.6
Y98m	43.8	Zr99	46.3	Y98m	52.7
Nb102	40.9	Y98m	43.8	Zr99	46.3
Y97m	34.7	Y96	43.4	Rb94	35.4
I	I	Y97	42.2	Y97m	34.4
Rb94	24.5	Nb102m	36.8	I	I
Nb102m	14.6	I	I	Nb102m	16.8
Y96	2.8	Nb102	16.8	Y96	2.9





- Below are the dominant nuclides and their *beta* heat contribution at 4s after pulse for ²³⁵U_{th} in kW
- JENDL: Y96 reallocated to gamma and Nb102(m) switch
- Rb94 differences but suspiciously little Rb92 difference

Nuclide	ENDF/B-VII.1	Nuclide	JENDL-4.0	Nuclide	JEFF3.2/3.1.1
Y96	116	Rb92	109	Y96	118
Rb92	107	Y96	95.8	Rb92	107
Zr99	89.2	Zr99	93.8	Zr99	84.6
Nb100	84.9	Nb100	82.8	Nb100	82.9
Cs142	71.0	Nb102m	71.4	Cs142	70.6
Zr101	61.5	Cs142	70.6	Zr101	61.5
I	I	Zr101	62.5	Nb102	60.6
Nb102	45.0	I	I	I	I
Rb94	26.1	Rb94	35.0	Rb94	40.0
Nb102m	14.6	Nb102	18.3	Nb102m	18.3





- Comparison with gamma shows clear discrepancies
- Nota bene again no Lowell data included in Tobias
- Better simulation with TAGS results, recently added in JENDL 4.0 and ENDF/B-VII.1, not JEFF-3.1.1 decay files !!





Dominant nuclide heat production for ²³⁹Pu_{th}

- Below are the dominant nuclides and their *gamma* heat contribution at 800s after pulse for ²³⁹Pu_{th} in kW
- Again Tc 104/5 different feeding for JEFF-3.1.1
- Sr93 jumps by 30% between ENDF and JENDL

Nuclide	ENDF/B-VII.1	Nuclide	JENDL-4.0	Nuclide	JEFF3.2/3.1.1
Tc104	93.8	Tc104	93.8	Tc104	54.9
Tc105	59.5	Tc105	59.6	Sr93	44.6
Mo101	44.5	Mo101	45.9	Mo101	44.5
Sr93	53.6	Sr93	40.6	Y95	29.5
Y95	33.1	Y95	30.0	Xe138	28.7
Xe138	28.8	Xe138	28.8	Cs138	26.9
Cs138	27.0	Cs138	27.0	Ba142	26.7
Ba142	26.7	Ba142	26.5	Tc105	21.8



Dominant nuclide heat production for ²³⁹Pu_{th}

- Below are the dominant nuclides nuclides and their *beta* heat contribution at 800s after pulse for ²³⁹Pu_{th} in kW
- Tc differences reflected in beta
- Suspiciously little difference in Sr93 beta, given gamma

Nuclide	ENDF/B-VII.1	Nuclide	JENDL-4.0	Nuclide	JEFF3.2/3.1.1
Tc102	64.3	Tc102	63.8	Tc102	64.2
Cs139	54.8	Cs139	54.6	Cs139	55.0
Y95	37.4	Y95	38.9	Tc104	46.3
Y94	37.2	Y94	37.1	Tc105	42.6
Tc104	27.0	Tc104	24.7	Y95	38.9
Tc105	24.9	Tc105	23.3	Y94	37.2
I	I	I	I	I	I
Sr93	15.9	Sr93	15.5	Sr93	16.0





- All fast fission results from YAYOI reactor by Akiyama et al
- Simulation using 400 keV pulse to access fast fission nFY
- Below are MeV/fission of ²³⁸U_f pulse gamma and C/E
- Discrepancies after ~2 hours (~1E4s) may be outside error?
 - No TAGS made for this time-period





Gamma discrepancies in fast fission vs Akiyama

- These are gamma C/E
- Other fast fission data shows similar disagreements
- Mainly due to beta/gamma (mis)allocation
- JEFF-3.1.1dd missing TAGS

JENDL4

10000

²³⁵U_f

1000

Time (s)

1.08

1.06

1.04

1.02

1

0.98

0.96 0.94

0.92

0.9

0.88

0.86

100

C/E Gamma Decay Heat





- Decay data application (nuclear fuel) responsible for purposeful and systematic overestimation in *e.g.* ANSI/ ANS-5.1
- Discrepancies between simulations with different dd show data is not accurate enough for sophisticated applications
- Uncanny agreement in γ, β and total heat values where individual nuclide contributions are substantially different
- Cumulative nFY should be re-examined to ensure no contamination with incomplete decay data
- Decay heat experiments are filled with complexity and care must be taken when making comparisons with simulations





- FISPACT-II capabilities:
 - Can calculate based on arbitrary pulses and longer irradiations
 - Any ENDF-6 formatted library can be used for calculations
 - Full uncertainty treatment if given by the data
 - Handles arbitrary combination of nFY and sFY, DD
 - Tracking heat contributions and pathways for nuclide production
- EASY-II with TENDL (or other capable library) has the ability to use fission yields of arbitrary incident neutron energy
 - Potentially required for correct beta feeding (and emitted neutrino spectrum)





- Are decay files 'evaluated' averages or are the averages calculated from the decay schemes??
- Appropriate decay scheme
- How to account and compensate for missing levels
- Decay data for isomers?

- High energy gamma lines transport further
- Low energy beta equates high energy anti-neutrino
- Missing gamma lines impact on doses





21st century multi-particle/system inventory code package for stockpile, fuel cycle stewardship, source terms, materials characterization and life cycle management for:

- Magnetic and inertial confinement fusion
- Fission Gen II, III+, IV plants and piles
- High energy and accelerator physics
- Medical applications, isotope production
- Earth exploration, Astrophysics
- Homeland security, material sciences
- . .
- Able to access rich, multifaceted nuclear data forms and their uncertainties.

http://www.ccfe.ac.uk/EASY.aspx

