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FISPACT-II: an advanced simulation platform for inventory and nuclear observables

"renaissance"

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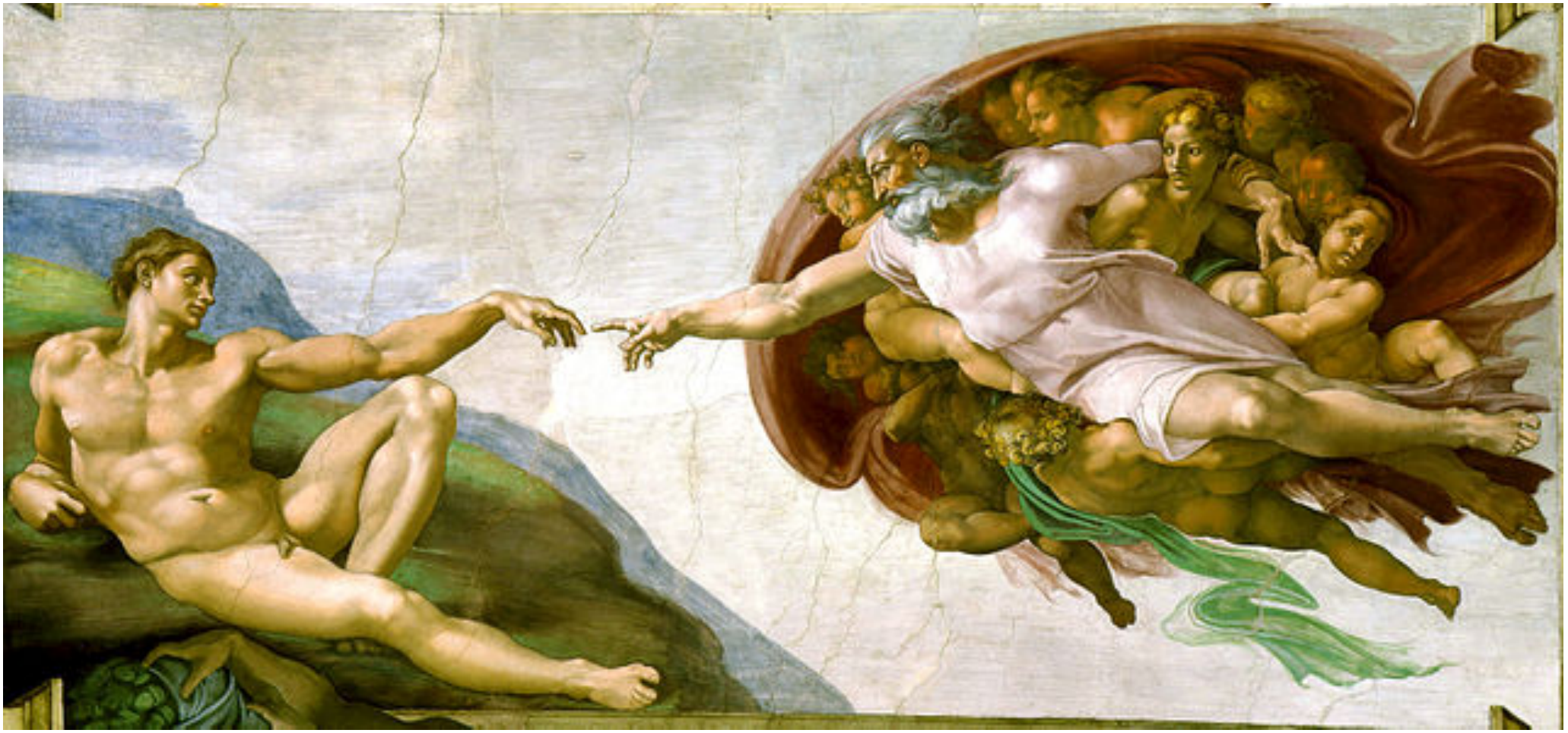
Italian renaissance



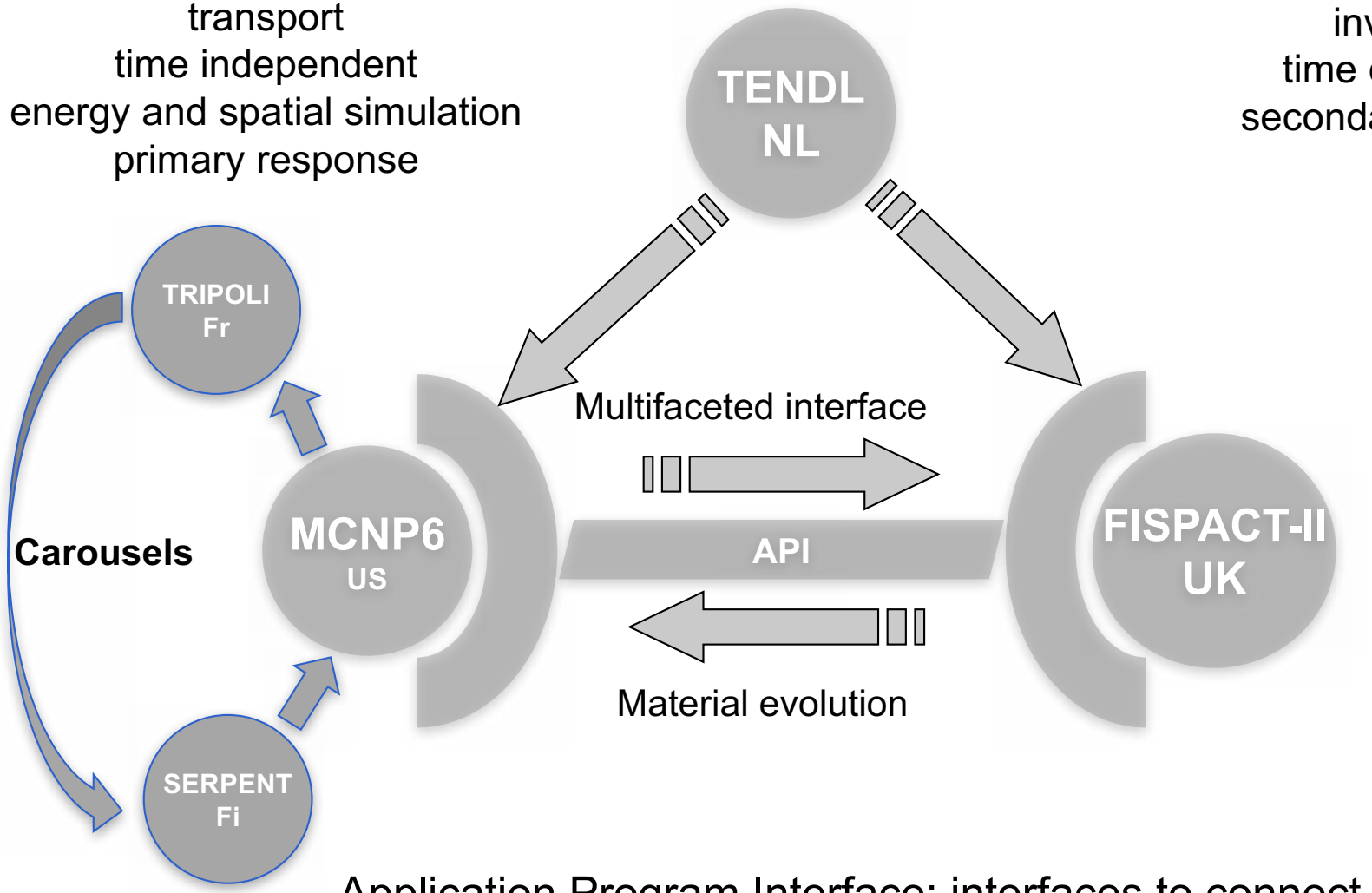
Michelangelo, (c. 1511) the Creation of Adam

Simulation in space, energy and time

Boltzmann equation
transport
time independent
energy and spatial simulation
primary response

Nuclear Data

Bateman equation
inventory
time dependent
secondary response



Application Program Interface: interfaces to connect Boltzmann and Bateman solvers for non-linear t- and T-dependent transport

Simulation framework

- FISPACT-II is a modern engineering prediction tool for activation-transmutation, depletion inventories at the heart of the an enhanced multi-physics platform that relies on the TALYS collaboration to provide the nuclear data libraries.

- All nuclear data application forms are handled by NJOY (LANL), PREPRO (LLNL) and CALENDF (UKAEA)

- d, p, α, γ, n-Transport Activation Library: TENDL-2015 from the TENDL collaboration, but also ENDF/B, JENDL, JEFF, CENDL and GEFY

FISPACT-II resources

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UKAEA-R(11)11 Issue 8
December 2016

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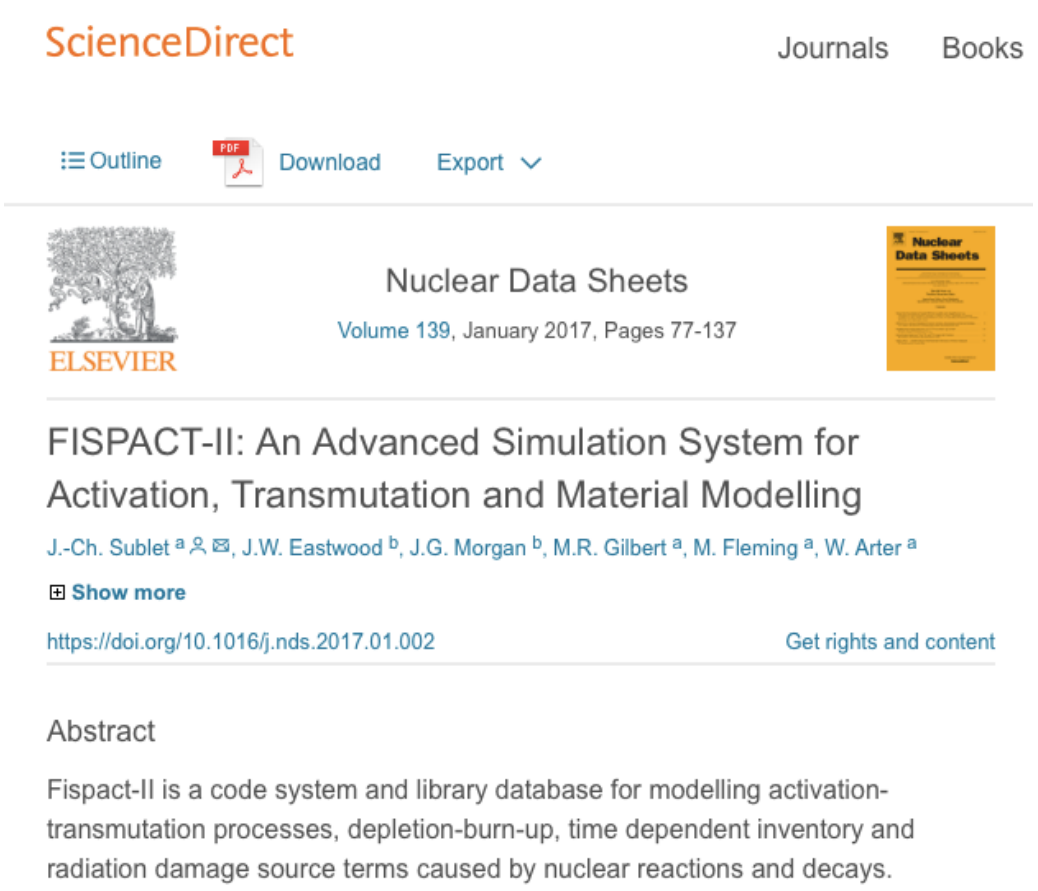
Mark R. Gilbert

The FISPACT-II User Manual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Nuclear Data Sheets

Volume 139, January 2017, Pages 77-137

FISPACT-II: An Advanced Simulation System for Activation, Transmutation and Material Modelling

J.-Ch. Sublet [a], J.W. Eastwood [b], J.G. Morgan [b], M.R. Gilbert [a], M. Fleming [a], W. Arter [a]

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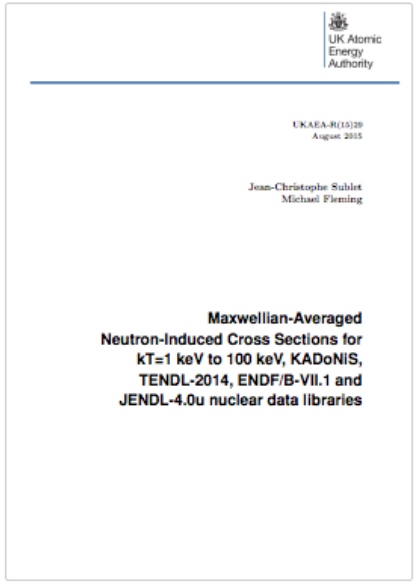
Abstract

Fispact-II is a code system and library database for modelling activation-transmutation processes, depletion-burn-up, time dependent inventory and radiation damage source terms caused by nuclear reactions and decays.

http://fispact.ukaea.uk/
http://www.sciencedirect.com/science/article/pii/S0090375217300029

FISPACT-II resources

- FISPACT-II and libraries are subject of various validation reports:
  - CCFE-R(15)25 Fusion decay heat
  - CCFE-R(15)27 Integral fusion
  - CCFE-R(15)28 Fission decay heat
  - UKAEA-R(15)29 Astro s-process
  - UKAEA-R(15)30 RI/therm/systematics
  - UKAEA-R(15)35 Summary report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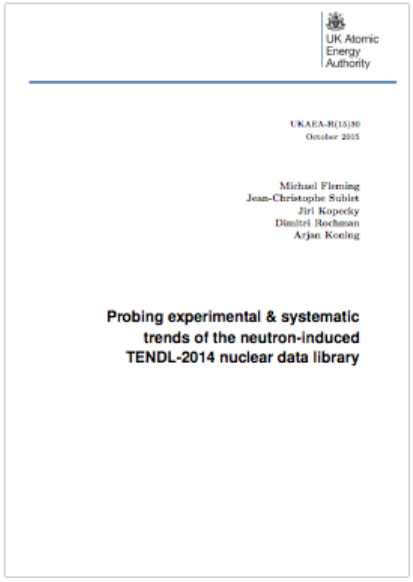
UKAEA-R(15)29
August 2015

Jean-Christophe Sublet
Michael Fleming

Maxwellian-Averaged Neutron-Induced Cross Sections for kT=1 keV to 100 keV, KADoNiS, TENDL-2014, ENDF/B-VII.1 and JENDL-4.0u nuclear data libraries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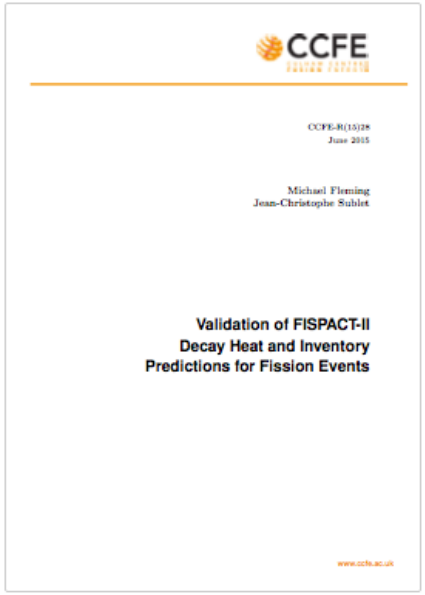
UKAEA-R(15)30
October 2015

Michael Fleming
Jean-Christophe Sublet
Jiri Kopecky
Dimitri Rochman
Arjan Koning

Probing experimental & systematic trends of the neutron-induced TENDL-2014 nuclear data library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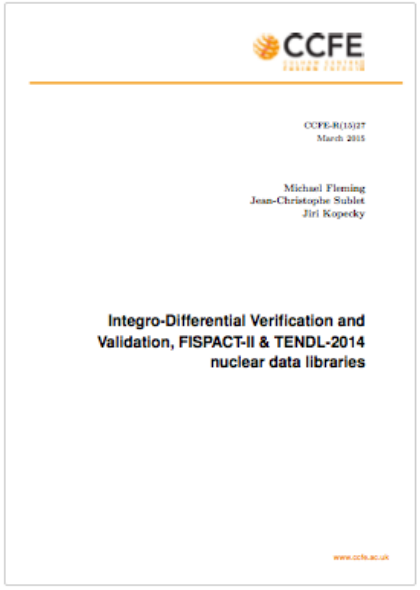
June 2015

Michael Fleming
Jean-Christophe Sublet

Validation of FISPACT-II Decay Heat and Inventory Predictions for Fission Events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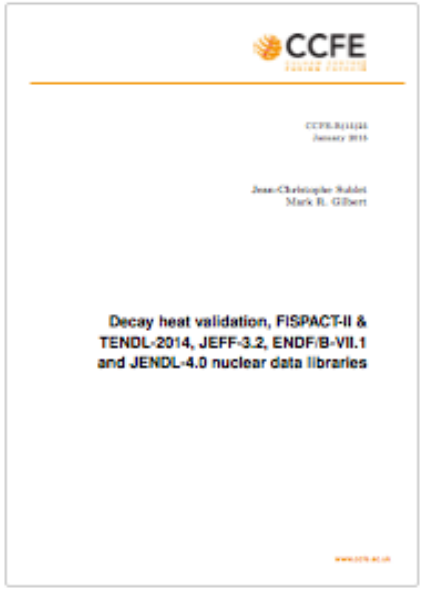
CCFE-R(15)27
March 2015

Michael Fleming
Jean-Christophe Sublet
Jiri Kopecky

Integro-Differential Verification and Validation, FISPACT-II & TENDL-2014 nuclear data libraries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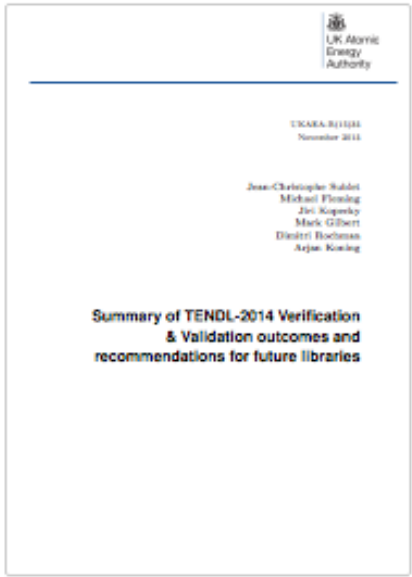
Mark R. Gilbert

Decay heat validation, FISPACT-II & TENDL-2014, JEFF-3.2, ENDF/B-VII.1 and JENDL-4.0 nuclear data libraries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Arjan Koning

Summary of TENDL-2014 Verification & Validation outcomes and recommendations for future libraries

Ordinary Differential Equation solver

Theory: H. Bateman, Cambridge 1910

- 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_{ij} is the constant for the decay of nuclide j to nuclide i

Analytical and Numerical Models

- Analytical models are mathematical solutions expressed in closed form. The solution to the equations used to describe the time evolution of a system can be expressed in terms of well-known mathematical functions whose numerical values can be computed accurately, reliably and quickly. Then the numerical values of solutions at any required times may be computed in principle, but not always in practice. For example, the accuracy of a solution may be severely limited by rounding error in floating-point arithmetic.

- Numerical models are used when analytical models are not available, or cannot be evaluated reliably. The approximate solution to a system of equations is obtained using an appropriate time-stepping procedure to evaluate the solution at a discrete sequence of desired times. Good procedures allow estimates of the numerical error to be obtained so that the accuracy of the solution is known. The mathematical solution is represented as a table of numbers generated by the numerical method and can be plotted as a graph.

Analytical and Numerical Models

- The choice of an appropriate numerical method for any particular problem cannot be made naively. Decades of research in the field of numerical analysis has yielded a wide variety of methods, each suited to specific classes of problems:

  Euler integration; exponential, matrix exponential, Newton-Krylov implicit integrators, Markovian chains, first to fifth-order Runge-Kutta, Chebyshev Rational Approximation, etc …

- In the case of the Bateman equations with constant coefficients:
  - an analytical solution is available in principle, but cannot be evaluated in practice
  - the solution can be expressed as a sum of exponential functions of time using the eigenvalues of the system matrix
  - unfortunately, these eigenvalues cannot be computed reliably because of ill-conditioning
  - if computable at all, the eigenvalues would take an unacceptably long time to evaluate

- For inventory calculations, key characteristics of the system of equations are
  - sparsity (most elements of the system matrix are zero)
  - stiffness (contrasting timescales between the rapid decay of some nuclides and the length of the desired time interval)

Rate equations: numerical aspects

- 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

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FISPACT-II advanced simulations

	FISPACT-II
Solver	Numerical - LSODES 2003
Incident particles	α, γ, d, p, n (5)
ENDF's libraries: TENDL-2015 & GEFY-5.3 ENDF/B-VII.1, JEFF-3.2, JENDL-4.0, CENDL-3.1 (~400 targets each)	✔ XS data (2809 targets) ✔ Decay data (3873 isotopes) ✔ nFY, sFY, otherFY ✔ Hazard, clearance indices, A2
Dpa, Kerma, Gas production, HE radionuclide yields	✔
PKA, recoil, emitted particles spectra	✔
Uncertainty quantification and propagation UQP	✔ Variance-covariance
Temperature (from reactor to astrophysics, plasma) 1 KeV ~ 12 million Kelvin	0, 294, 600, 900 K,…5, 30, 80 KeV
Self-shielding with probability tables **and/or** with resonance parameters	✔ Resolved and Unresolved Resonance Range
Energy range	1.0 10^{-5}eV – 30, 200 MeV, ..1GeV
Sensitivity	✔ Monte Carlo
Pathways analysis, routes of production	✔ multi steps
Thin, thick targets yields	✔

FISPACT-II features: ENDF's libraries

- Covariance information on neutron entrance channels, uncertainty
- Pathways analysis, production routes, dominant contributors
- Self-shielding effects: channels, isotopic, elemental

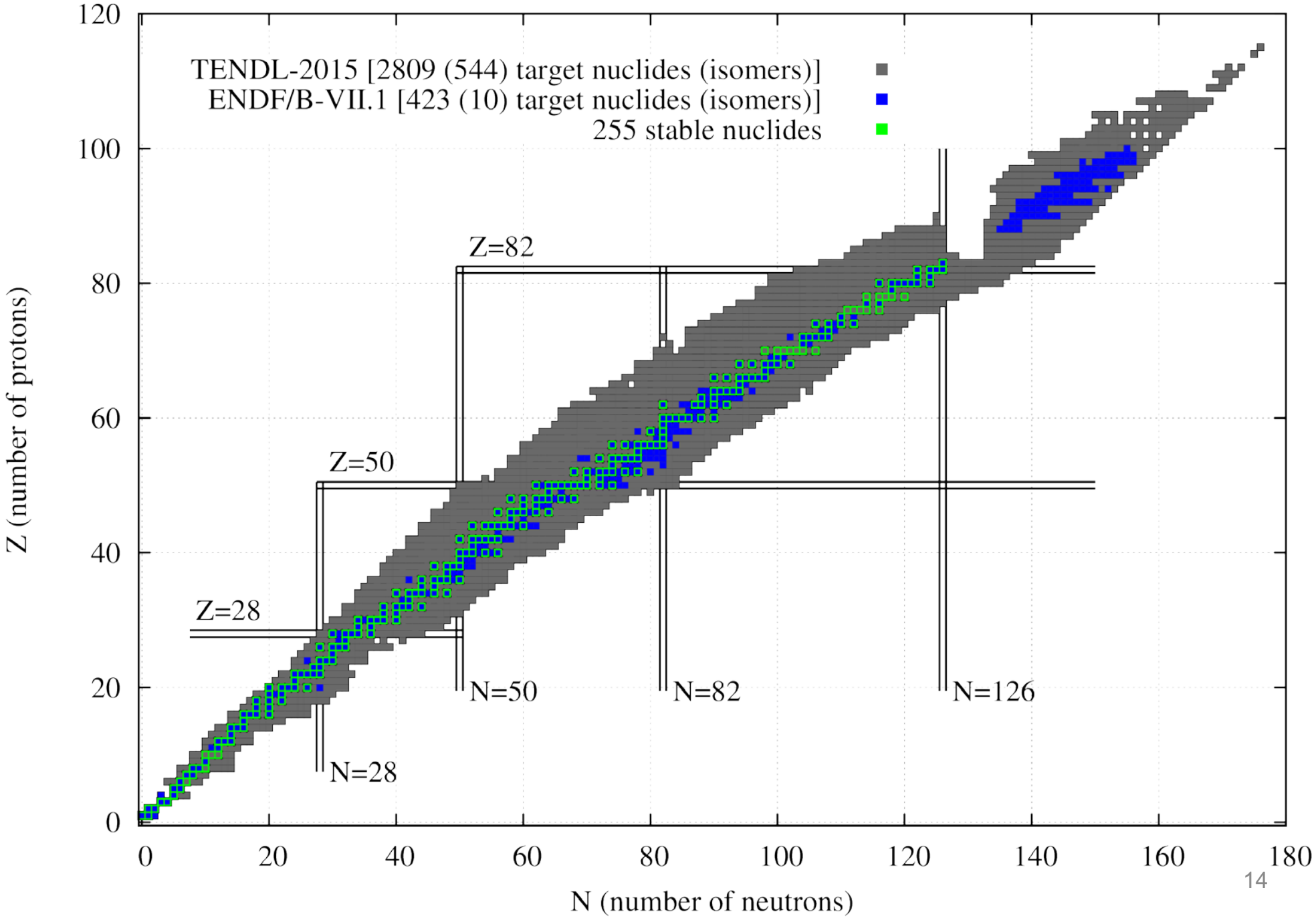
- Sensitivity analysis, (Monte Carlo)
- Isomeric states and branching ratio (γ, m, n, o, p, q,…., from RIPL)
- Consistent decay data and cross section data: energy levels

- DPA, Kerma (primary and secondary), gas and radionuclide production
- Temperatures: 0, 294, 600, 900 K,… and stellar 5 Kev, 30 KeV, 80 KeV (1 Kev = 12 10^6K)
- Thin, thick target yields

- V&V suites: fusion, fission, accelerator, astrophysics,..

For all nuclear applications

Isotopic targets



Processing steps: burnup, transmutation

- Multi-particle groupwise, multi-temperature libraries with NJOY12-099, PREPRO-2017, probability tables in the RRR & URR with CALENDF-2010
  - For the inventory code FISPACT-II
- From α, γ, p, d, n-TENDL-2017 & ENDF/B-VII.1, JEFF-3.2, JENDL-4.0u, CENDL-3.1
- FISPACT-II parses directly the TENDL's covariance complex information
- Transport and activation application libraries now stem from unique, truly general purpose files

FISPACT-II TENDL's libraries – 200 MeV

- n-tendl-2015, multi temperatures, 1102 groups library for 2809 targets
  - ✓ full set of covariance
  - ✓ probability tables in the RRR and URR
  - ✓ xs, dpa, kerma, gas, radionuclide production
  - ✓ PKA matrices for the stables

- JENDL-4.0u, ENDF/B-VII.1, JEFF-3.2, CENDL-3.1, 1102 groups libraries for circa 400 targets each

- γ-tendl-2015, 162 groups xs library, 2804 targets
- p-tendl-2015, 162 groups xs library, 2804 targets
- d-tendl-2015, 162 groups xs library, 2804 targets
- α-tendl-2015, 162 groups xs library, 2804 targets

FISPACT-II other libraries

- ✓ UKDD-2012, 3873 isotopes (23 decay modes; 7 single and 16 multi-particle ones)
- ✓ Ingestion and inhalation, clearance and transport indices libraries, 3873 isotopes
- ✓ GEFY 5.3, JEFF-3.1.1, UKFY4.2, ENDF/B-VII fission yields
- ✓ ENDF/B-VII.1 DD and FY
- ✓ JENDL-4.0 DD and FY

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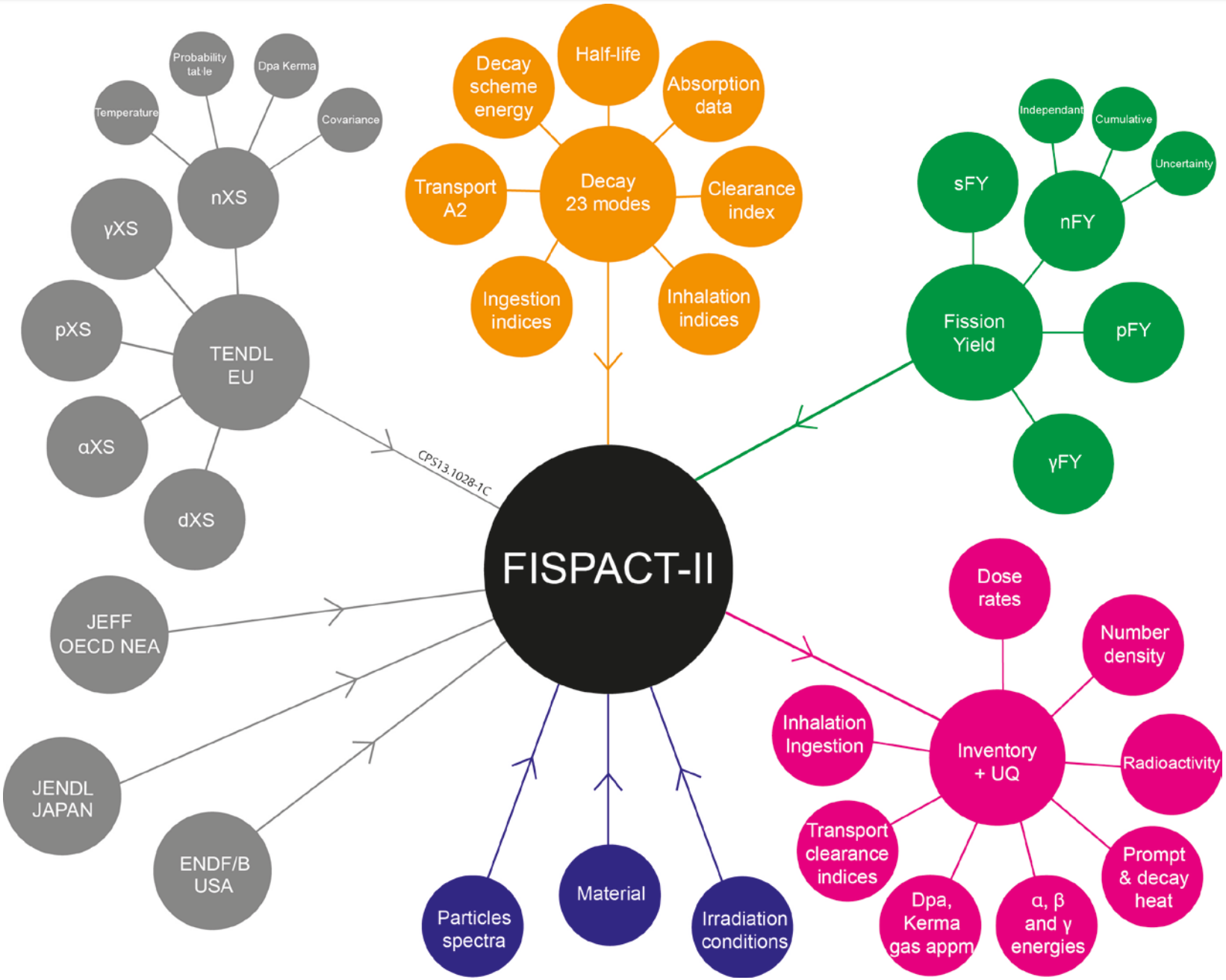
FISPACT-II &TENDL & ENDF/B, JENDL, JEFF, CENDL



FISPACT-II new features

Reaction rate uncertainty quantification and propagation, variance-covariance

FISPACT-II irradiation scenarios

- Single irradiation pulse followed by cooling
- Multiple irradiation pulses
  - changing flux amplitude
  - cooling
- Multi-step
  - changing flux amplitude and spectrum
  - changing cross-section (e.g., temperature dependence)
  - cooling
- Pathways and sensitivity for all cases

What FISPACT-II does

- Extracts and reduces nuclear and radiological data
- Solves rate equations for time evolution of inventory
- Computes and outputs derived radiological quantities
- Identifies and quantifies key reactions and decay processes:
  - dominant nuclides
  - pathways and uncertainty
  - Monte-Carlo sensitivity and uncertainty
  - reduced model calculations
- Uncertainty calculation
  - input cross-section and decay uncertainties
  - output uncertainties for all radiological quantities

Extract and reduce library data

- Condense run extracts from decay files:
  - decay constant λ
  - decay constant uncertainty Δλ
- Collapse constructs flux spectrum weighted averages:

- Library input
  - cross-section vs energy
  - covariances vs energy
  - flux spectrum vs energy

$$W_i = \frac{\phi_i}{\sum_{i=1}^{N} \Phi_i}$$

$$\overline{XS} = \sum_{i=1}^{n} W_i X_i$$

- Data used in code
  - collapsed cross-section $\overline{XS}$
  - collapsed uncertainty Δ

Covariance collapse

- reactions X and Y
- energy bins i and j $\in$ [1,N] with N = 709
- uses Cov (X_i,Y_j) for X ≠ Y only in Monte-Carlo
- collapse Cov (X_i,X_j) to get uncertainty Δ for $\overline{X}$

$$var = \sum_{i=1}^{N}\sum_{j=1}^{N} W_i W_j Cov(X_i, X_j); \qquad \Delta = \{1|3\}\sqrt{var}/\bar{X}$$

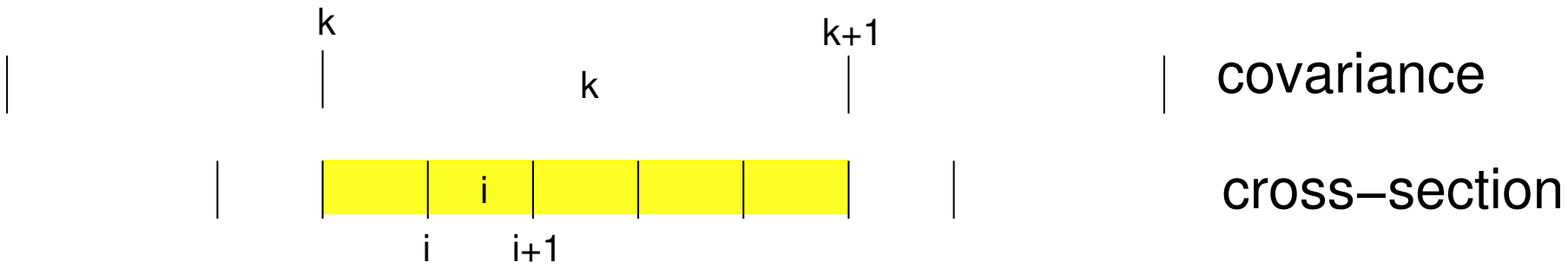
1 TENDL, 3 EAF

- Collapse Cov(X_i,Y_j) to get Cov($\overline{X}$, $\overline{Y}$) for X ≠ Y
- Cov data in ENDF file 33 & 40, NI type LB=1, 5, 6
- Cov data in wider energy bins k $\in$ [1, M], M ~ 40

Covariance, variance

The projection operator S_i^k maps cross-section energy bins to covariance energy bins

$$S_i^k = \begin{cases} 1 & \text{bin i in bin k} \\ 0 & \text{otherwise} \end{cases}$$



The ENDF style covariance data forms, different LB's are read directly without the need of pre-processing

Covariance, variance

Using S_i^k, the formula to construct estimates of the covariance matrix are as follows:

$$LB = 1: \quad Cov(X_i, X_j) = \sum_{k=1}^{M} S_i^k S_j^k F_k X_i X_j$$

➔➔

$$LB = 5: \quad Cov(X_i, Y_j) = \sum_{k=1}^{M} \sum_{k'=1}^{M} S_i^k S_j^{k'} F_{kk'} X_i Y_j$$

➔➔

$$LB = 6: \quad Cov(X_i, Y_j) = \sum_{k=1}^{M} \sum_{k'=1}^{M'} S_i^k S_j^{k'} F_{kk'} X_i Y_j$$

$$LB = 8: \quad Cov(X_i, X_j) = \sum_{k=1}^{M} S_i^k S_j^k 1000 F_k \quad (Koning)$$

$$(or = \sum_{k=1}^{M} S_i^k \delta_{ij} 1000 F_k)$$

The LB=1 case is the one that was applied to the computation of Δ for the EAF's libraries

Uncertainty in FISPACT-II

- Given$\{\overline{XS}, \lambda\}$
  - select irradiation scenario
  - solve for radiological quantities

- Use $\{\Delta X, \Delta\lambda\}$ to estimate uncertainties
  - method 1: pathways to dominant nuclides
  - method 2: Monte-Carlo sensitivity
  - method 3: reduced model Monte-Carlo sensitivity

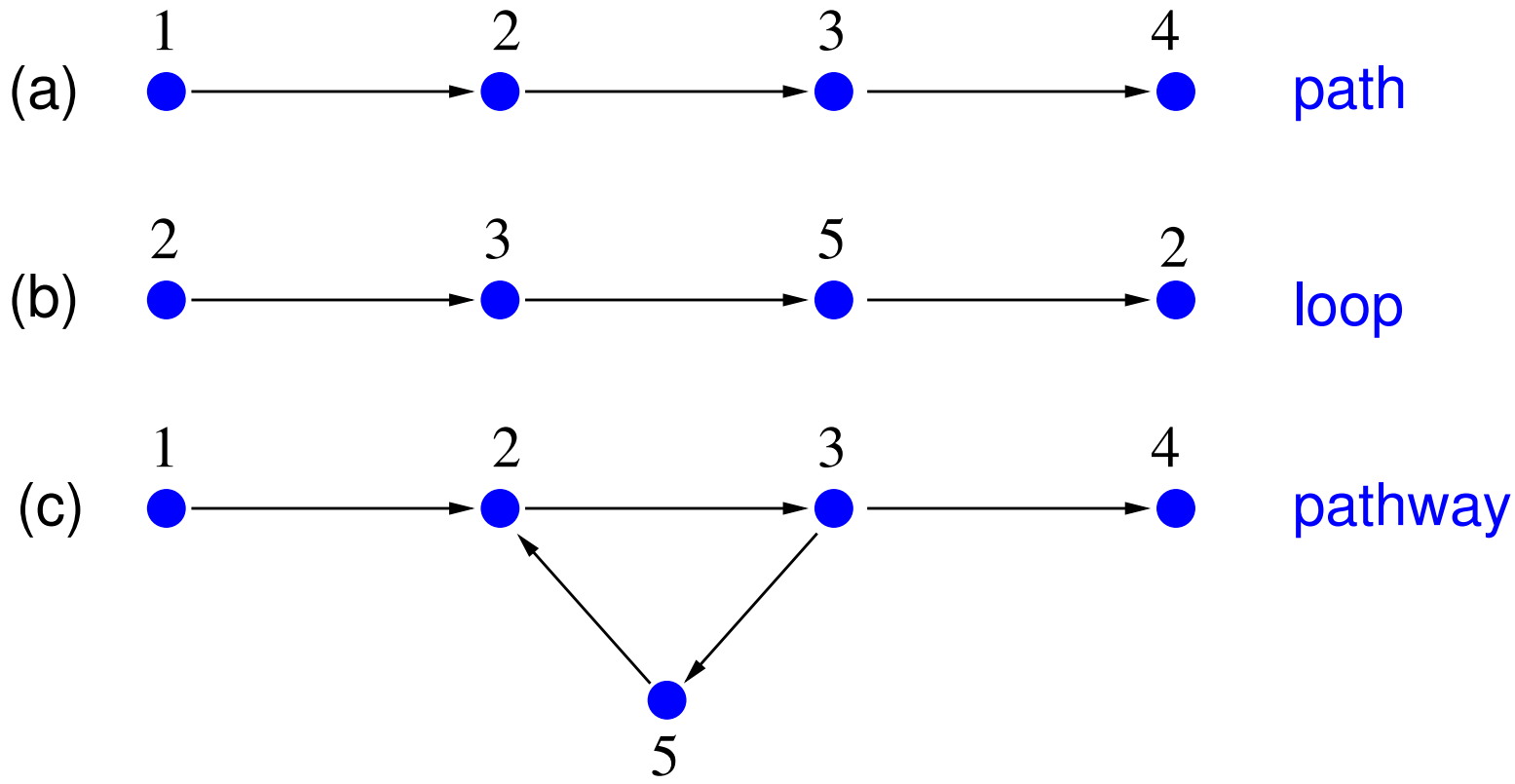
Uncertainty in FISPACT-II

- Pathways are used to identify the dominant contributors to the activation products for the specific irradiation scenario under consideration.
- This makes the calculation of uncertainties more practicable for all methods (random-walk approximation and Monte-Carlo).
- The standard uncertainty output uses a random-walk approximation to estimate error bounds.
- This estimate is much quicker than Monte-Carlo, but is likely to give larger bounds since it ignores many possible correlations.

Uncertainty from pathways

- given initial inventory and irradiation scenario
- sort dominant nuclides at end of irradiation phase
  - `topxx` (=20) controls number
  - 8 categories - activity, heat production, dose, etc.
- construct pathways from initial to dominant nuclides
  - `path_floor` (=0.005) `and loop_floor` (=0.01)
  - iterate on single-visit breadth-first search tree
- compute inventory contributions of pathways
- construct error estimate

Pathways



- keep pathways providing > `path_floor` of target inventory
- keep loop providing > `loop_floor` of pathway inventory

Error estimate

$$Q = \sum_{t \in S_t} q_t; \quad (\Delta Q)^2 = \sum_{t \in S_t} \left(\frac{\Delta N_t}{N_t} \right)^2 q_t^2$$

$$(\Delta N_t)^2 = \sum_{p \in S_o} \Delta_{tp}^2 N_{tp}^2 + \sum_{a \in s_{sa}} \left(\sum_{p \in S_a} |\Delta_{tp}| N_{tp} \right)^2$$

$$\Delta_{tp}^2 = \sum_{e \in S_e} \sum_{r \in S_r} \left[\frac{R_r \Delta_r}{R_e} \right]^2 + \sum_{e \in D_e} \left[\frac{\Delta \lambda_e}{\lambda_e} \right]^2$$

- N_t (atoms) and q_t (radiological quantity) from rate equation
- Δ_{tp}, N_{tp}, ΔN_t from pathways
- R_r and R_e pulse averaged reaction rates
- reactions uncorrelated, fission correlated

Pathways and uncertainty output example

```
                                        UNCERTAINTY ESTIMATES (cross sections only)
                                        -------------------------------------------

Uncertainty estimates are based on pathway analysis for the irradiation phase
Total Activity is         1.25070E+14  +/-  8.52E+11  Bq.     Error is   6.81E-01 % of the total.

Total Heat Production is  3.60059E-02  +/-  3.09E-04  kW.     Error is   8.60E-01 % of the total.

Total Gamma Dose Rate is  5.63098E+04  +/-  5.04E+02  Sv/hr.  Error is   8.95E-01 % of the total.

Total Ingestion Dose is   1.38528E+05  +/-  1.17E+03  Sv.     Error is   8.45E-01 % of the total.
...

 Target nuclide Sc 44     99.557% of inventory given by  8 paths
 --------------------

 path  1  20.048% Ti 46 ---(R)--- Sc 45 ---(R)--- Sc 44 ---(S)---
                        98.16%(n,np)   100.00%(n,2n)
                         1.84%(n,d)

 path  2  12.567% Ti 46 ---(R)--- Sc 45 ---(R)--- Sc 44m---(b)--- Sc 44 ---(S)---
                        98.16%(n,np)   100.00%(n,2n)   100.00%(IT)
                         1.84%(n,d)                      0.00%(n,n)

 path  3  11.143% Ti 46 ---(R)--- Sc 45m---(d)--- Sc 45 ---(R)--- Sc 44 ---(S)---
                        96.62%(n,np)   100.00%(IT)     100.00%(n,2n)
                         3.38%(n,d)
...
```

Using LB = 6 data

- The TENDL library contains MF=33, LB=6 data for different reactions X_1, X_2, ... for a given parent, i.e., p(n, X_1)d_1, p(n, X_2)d_2, ...
- These covariance data cov(X_1,X_2) for X_1, X_2 are stored as fractional values f^{X1X2} and are tabulated in the same energy bins as used respectively for the LB=5 covariance data f^{X1X1}, f^{X2X2} for reactions X_1, X_2
- If the `COVARIANCE` keyword is used, FISPACT-II reads these data for all energy bins k and l and corrects for any instances where

$$\left| \frac{f_{kl}^{X_1X_2}}{\sqrt{f_{kk}^{X_1X_1} f_{ll}^{X_2X_2}}} \right| > 1$$

Using LB = 6 data

- Then the code uses the corrected data to compute collapsed covariance cov(X_1,X_2). Covariances are mapped to MF=10 by assuming that all isomeric daughters of a given pair of reactions with rates X_1, X_2 have the same collapsed correlation function, corr(X_1,X_2).
- Tables of all reactions which have covariance data and their collapsed covariances and correlations are printed by the collapse run. Inspection of these data will show those cases where the assumption of zero correlation between reactions of a given parent is not good.
- The effect of non-negligible correlations on uncertainties may be introduced into Monte-Carlo sensitivity calculations by choosing distributions of sample cross-sections to have the same variances and covariances as given by the TENDL data.

Uncertainty from sensitivity calculation

- reference run + S inventory calculations
- independent $\{X_i^s$; i = 1,...,I; s = 1,...,S$\}$
- dependent $\{Y_j^s$; j = 1,...,J; s = 1,...,S$\}$
- independent variables selected using random numbers
  - normal, log-normal, uniform, log-uniform
  - means $\langle X_i \rangle$ and standard deviations $\langle \Delta X_i \rangle$
- compute summary results:
  - means
  - standard deviations
  - Pearson correlation coefficients
- output full data for post-processing

Monte Carlo approach to sensitivity analysis

- output mean and standard deviation

$$\bar{X}_i = \frac{1}{S}\sum_{s=1}^{S} X_i^s \qquad \Delta X_i = \sqrt{\frac{1}{S-1}\sum_{s=1}^{S}[(X_i^s)^2 - \bar{X}_i^2]}$$

$$\bar{Y}_j = \frac{1}{S}\sum_{s=1}^{S} Y_j^s \qquad \Delta Y_j = \sqrt{\frac{1}{S-1}\sum_{s=1}^{S}[(Y_j^s)^2 - \bar{Y}_j^2]}$$

- Pearson correlation coefficient

$$r_{ij} = \frac{\sum_s X_i^s Y_j^s - S\bar{X}_i\bar{Y}_j}{\Delta X_i \Delta Y_j}$$

- controlled by keywords `SENSITIVITY`, `MCSAMPLE`, `MCSEED`, `COVARIANCE`

Sample sensitivity output

```
 Base cross section data
 index          parent                          daughter              sigma      sigma_unc
     i   zai    nuc_no  name      i   zai    nuc_no  name             cm**2
    1  220460     233   Ti 46      210460     219   Sc 46       0.39039E-25  0.35942E-01
    2  220460     233   Ti 46      210461     220   Sc 46m      0.10142E-25  0.35942E-01
    3  220480     235   Ti 48      210480     222   Sc 48       0.11049E-25  0.87272E-02
...
 Output nuclides
    j    zai    nuc_no  name
    1  210460     219   Sc 46
    2  210470     221   Sc 47
    3  210480     222   Sc 48
...
 Normal, x cutoff = [ -3.0000    ,  3.0000    ] std dev
```

← Normal random sampling

```
    j   atoms_base   atoms_mean    atoms_unc
    1  2.50290E+20  2.49955E+20  2.46164E-02
    2  7.99801E+18  7.99665E+18  1.68690E-03
    3  9.91006E+18  9.90588E+18  8.55649E-03
...
 Correlation coefficients
   j\i       1            2            3            4
     1  9.66468E-01   - - - -      - - - -      - - - -
     2   - - - -      - - - -      - - - -     9.99810E-01
     3   - - - -      - - - -     1.00000E+00   - - - -
     4   - - - -      - - - -     9.99993E-01   - - - -
     5   - - - -      - - - -      - - - -    -9.99911E-01
     6   - - - -      - - - -    -9.60898E-01   - - - -
     7 -9.66478E-01   - - - -      - - - -      - - - -
```

← reactions

↑ output nuclides

Uncertainty from reduced models

- UKDD-2012 decay - 3873 nuclides
- calculation includes all nuclides in master index
- `INDEXPATH` generates reduced master index from pathways
  - typically few 10s of nuclides
  - number adjustable by pathway parameters
- reduced master index run vs full run to validate discards
- Monte-Carlo sensitivity for reduced master index runs
  - faster + comparable answers

FISPACT-II new features

Self shielding of resonant channels

- Probability tables, sub-group method
- High fidelity resonances

Self shielding of resonant channels

CALENDF probability tables are used to model dilution effects in the computation of the effective cross-sections

cal-mt	description	mt in set
2	elastic scattering	2
101	absorption (no outgoing neutron)	102 103 107
18	fission total	18
4	inelastic scattering (emitting one neutron)	4 11
15	multiple neutron production (excluding fission)	5 16 17 37

$\sigma_{eff}(x, n) = \sigma_{eff}(g, x, n)$ and $p(x, n) = p(g, x, n)$

where
g = energy group number
x = macro-partial (or total) index
n = quadrature index

Cross section, PT distribution, discretization

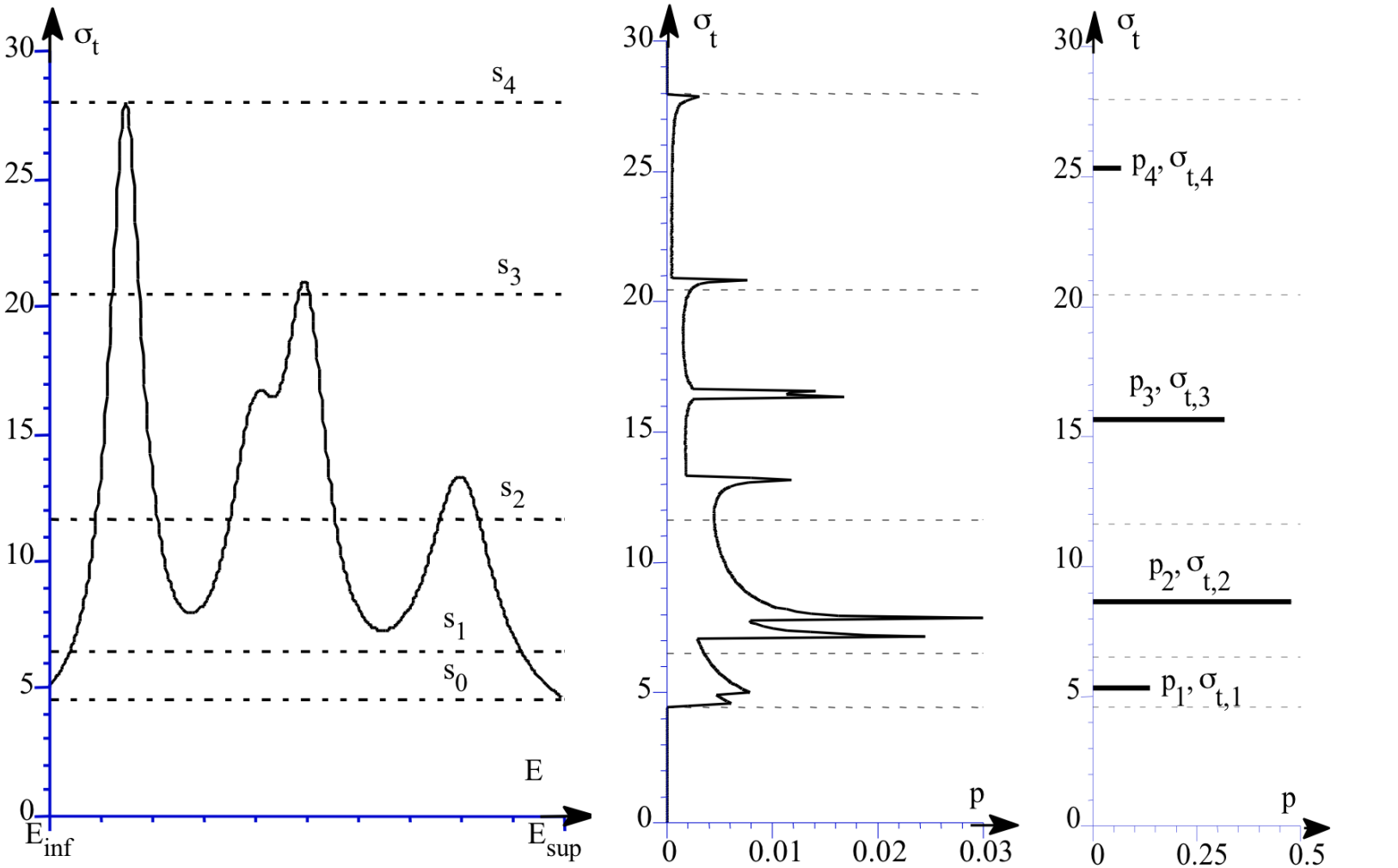


Fig. 1a Cross section versus energy **1b** Exact PT distribution **1c** PT discretisation

$$\frac{1.}{G}\int_{E_{\inf}}^{E_{\sup}} \sigma_t^n(E)dE \quad = \quad \int_{\sigma_{\min}}^{\sigma_{\max}} p(\sigma_t)\sigma_t^n d\sigma_t \quad = \quad \sum_{i=1}^{i=N} p_i \ \sigma_{t,i}^n$$

Padé approximant and Gauss Quadrature

The moments having been computed, the probability table is established:

$$I(z) = \int \frac{p(x)}{1 - zx} dx = \underbrace{M_0 + M_1 z + M_2 z^2 + \ldots\ldots + M_{2N-1} z^{2N-1}}_{2N\ moments} + R_{2N} z^{2N}$$

$$= \underbrace{\frac{b_0 + b_1 z + b_2 z^2 + \ldots\ldots + b_{N-1} z^{N-1}}{1 + a_1 z + a_2 z^2 + \ldots\ldots + a_N z^N}}_{Q_{N,N-1} = PADE\ approximant} + R'_{2N} z^{2N}$$

$$= \frac{b_0 + b_1 z + \ldots\ldots + b_{N-1} z^{N-1}}{\prod_{i=1}^{N} (1 - z x_i)} + R'_{2N} z^{2N} = \underbrace{\sum_i \frac{p_i}{1 - z x_i}}_{p_i, x_i = quad.table} + R'_{2N} z^{2N}$$

The second line is the Padé approximant that introduces an approximate description of higher moment order

Effective cross section and moment

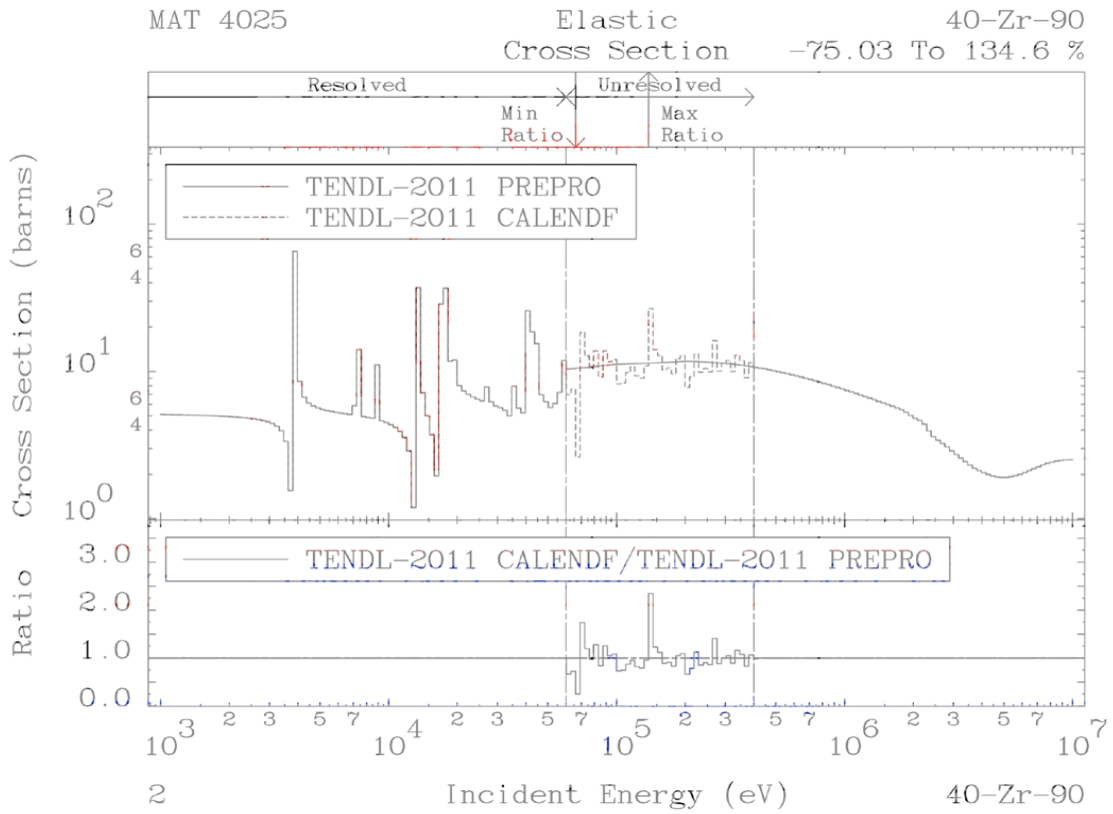
The effective cross section can be calculated from either the pointwise cross section or the probability table as follows:

$$\sigma_{x,eff,quad.}(\sigma_d) = \frac{\sum_{i=1}^{i=N} \frac{p_i \sigma_{x,i}}{\sigma_{t,i} + \sigma_d}}{\sum_{i=1}^{i=N} \frac{p_i}{\sigma_{t,i} + \sigma_d}}$$

When the dilution is infinite this formula becomes:

$$\sigma_{x,eff,quad.} = \sum_{i=1}^{i=N} p_i \sigma_{x,i}$$

Effective cross sections comparison



From 0.1 eV to the end of the URR

Uniquely accessible SSF's in the URR !!

Self Shielding Factor

The probability tables from CALENDF are used in conjunction with fine 709 or 1102 group data. They are given at 3 temperatures: 293.6, 600 and 900 Kelvin

Dilution

The dilution d(p; g) for a given nuclide p and energy group g is computed using a weighted sum over all the nuclides, q = 1;Q in the mixture. The first approximation for the fraction f_q uses the total cross-sections :

$$d^{(0)}(p,g) = \sum_{\substack{q=1 \\ p \neq q}}^{Q} \frac{f_q \sigma^{LIB-tot}(q,g)}{f_p}$$

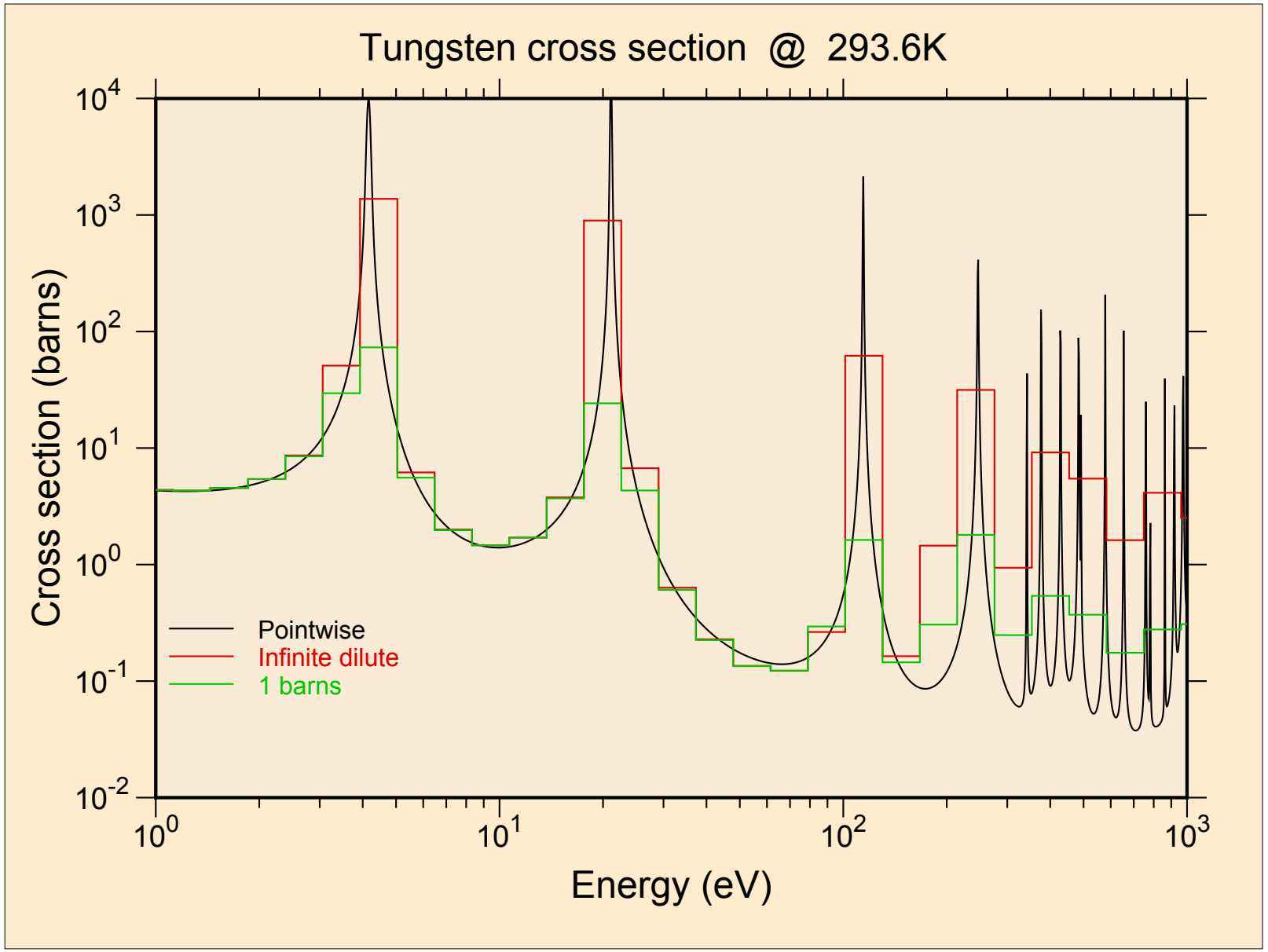
where

$$\sigma^{LIB-tot}(p,g) = \sum_{y=1}^{Y} \sigma^{LIB}(p,g,y)$$

Over the energy range for which the probability table data are available, the above approximation is iteratively refined using:

$$\begin{aligned} S^{(i)}(g) &= \sum_{q=1}^{Q} f_q \sigma^{LIB-tot}(q,g) \left(\frac{\sigma^{tot}(q,g,d^{(i)}(q,g))}{\sigma^{tot}(q,g,\infty)} \right) \\ d^{(i+1)}(p,g) &= \frac{S^{(i)}(g)}{f_p} - \sigma^{LIB-tot}(p,g) \left(\frac{\sigma^{tot}(p,g,d^{(i)}(p,g))}{\sigma^{tot}(p,g,\infty)} \right) \end{aligned}$$

Effective cross section: dilution effects



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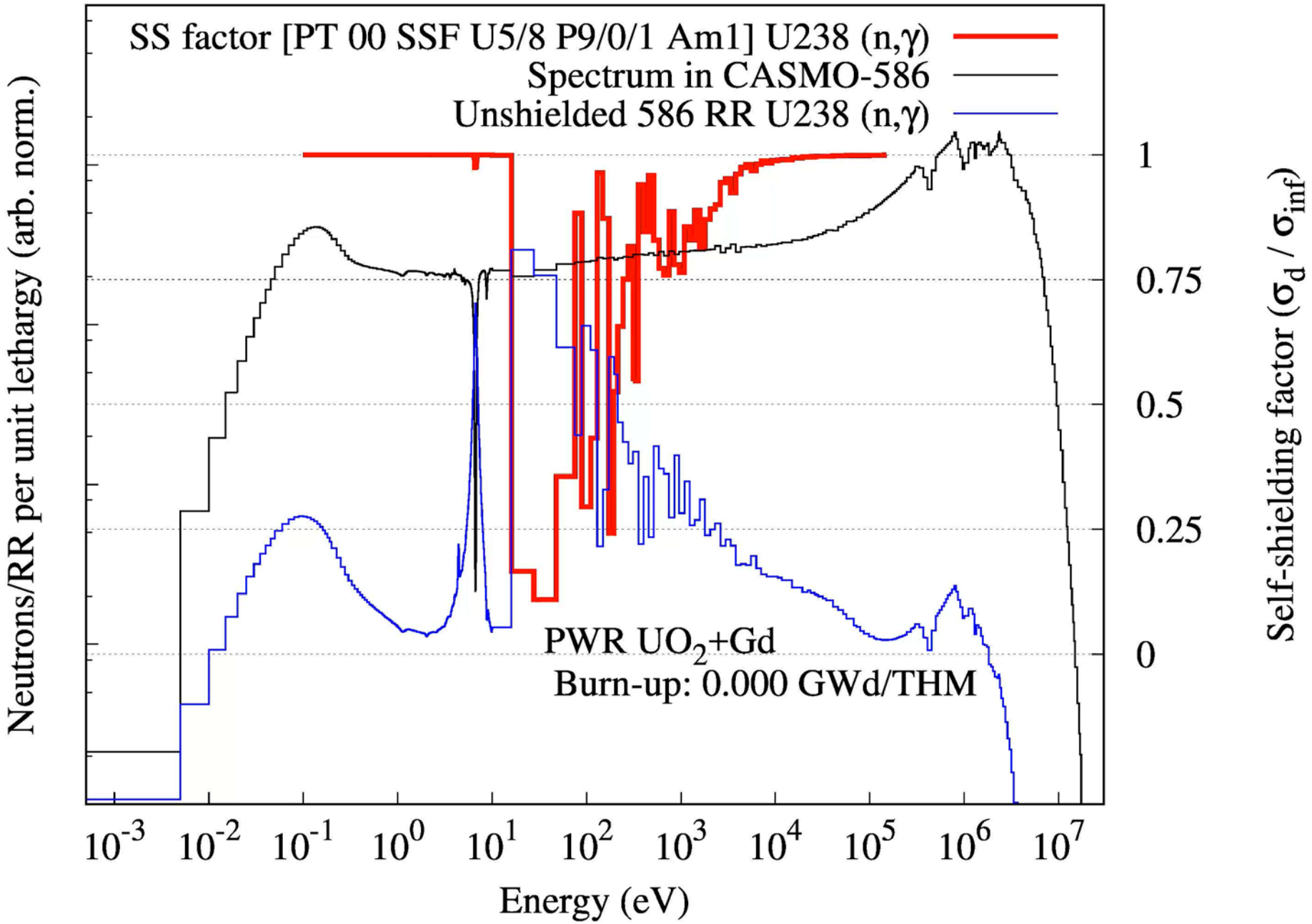
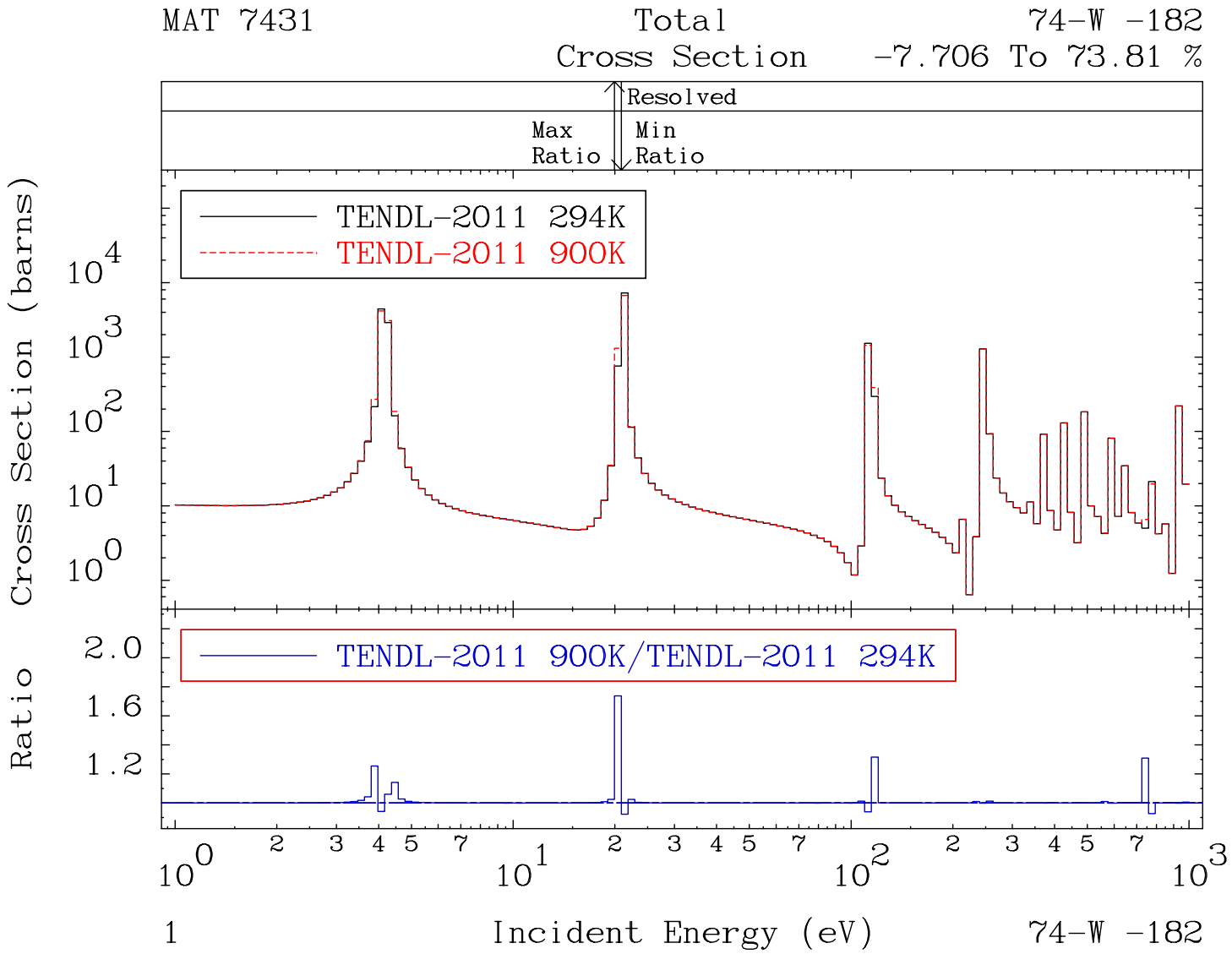
LWR UO_2 + Gd assembly



Temperature effect



Giant resonances dominate the reaction rate

The effect is not negligible around the resonances

FISPACT-II new features

Self shielding of resonant channels

- thin and thick target yields
- High fidelity resonance

Neutron self-shielding model

- thin and thick target yields
- accounts approximately for target geometry
- applicable to thick targets
- handles foils, wires, spheres and finite cylinders
- uses one physical length scale to represent the target: the "effective length" y

Type ID	Geometry	Dimension(s)	Y
1	foil	thickness (t)	y=1.5t
2	wire	radius (r)	y=2r
3	sphere	radius (r)	y=r
4	cylinder	radius (r), height (h)	y=1.65rh(r+h)

Epithermal Neutron Self-shielding Model

- theory of radioisotope production
- production rates and cross-sections
- saturation factors and practical yields

- model uses resonance parameters from the Resolved Resonance Range
- model includes the effects of neutron loss through radiative capture
- model includes effects of neutron energy diffusion through elastic scattering

Model development, first step (1)

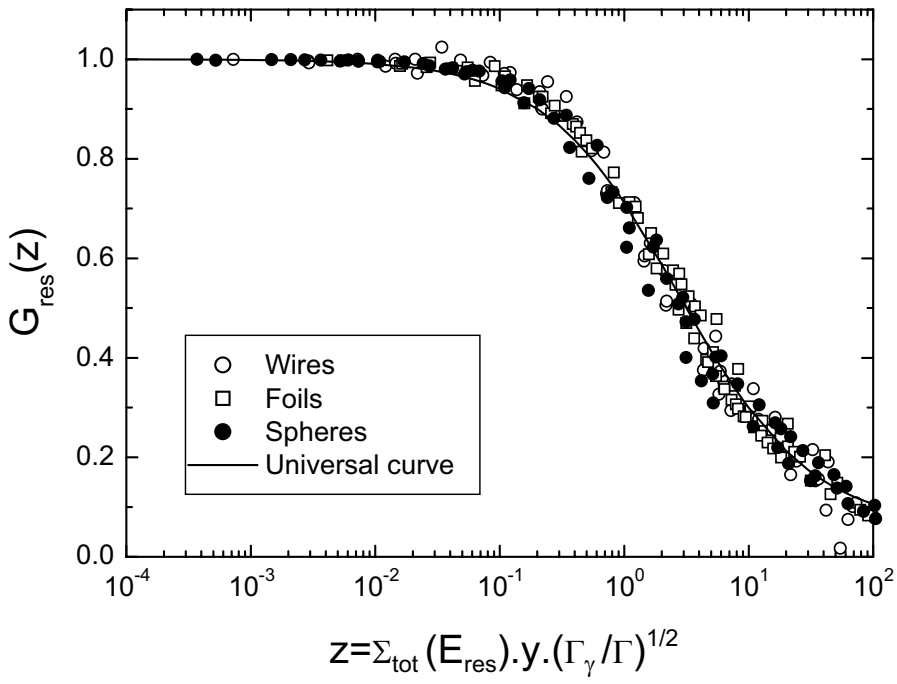
- one resonance in a pure target
- dimensionless parameter to combine the physical effective length with the nuclear parameters

$$z = \sum_{tot}(E_{res})y\sqrt{\frac{\Gamma_\gamma}{\Gamma}}$$

- where
  - $\Sigma_{tot}(E_{res})$ is the macroscopic cross-section at the energy E_{res} of the resonance peak
  - Γ_γ is the radiative capture width
  - Γ is the total resonance width
  - y “effective length”
- Self-shielding factor G_{res} is defined in terms of z only

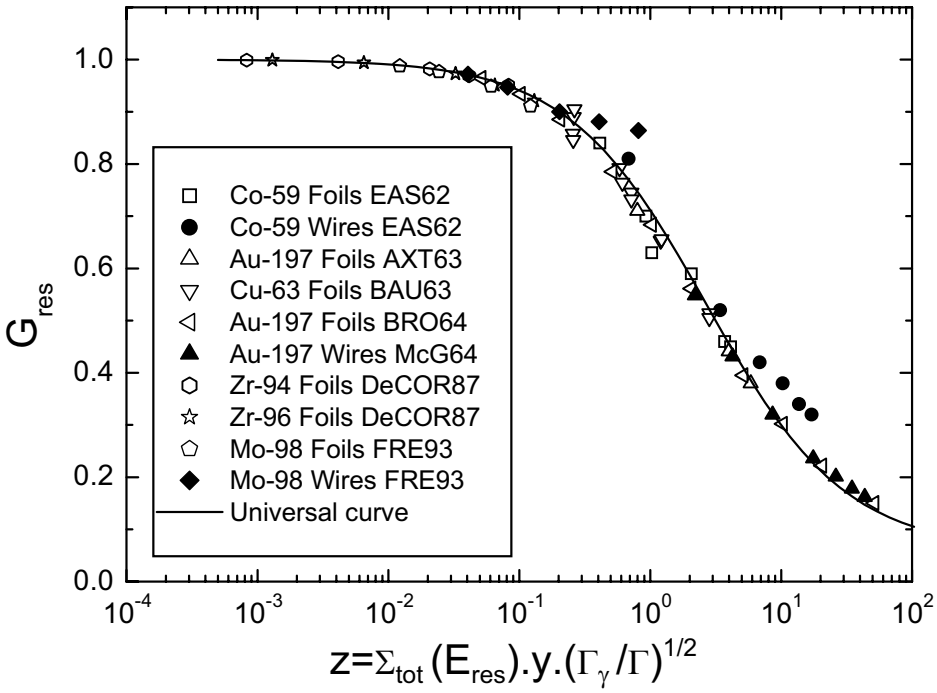
Model development, first step (1)

Baumann, 1963; Yamamoto and Yamamoto, 1965; Lopes, 1991



Target geometry

Experimental self shielding factor



Model development, first step (2)

$$G_{res}(z) = \frac{A_1 - A_2}{1 + \left(z / z_0 \right)^p} + A_2$$

- this is the “universal sigmoid curve” for the model
- the parameters have been determined empirically to be a good fit to experimental data
- preferred values are:
  - A1 = 1.000 ± 0.005
  - A2 = 0.060 ± 0.011
  - Zo = 2.70 ± 0.09
  - p = 0.82 ± 0.02

Model development, second step

- extend model to a group of separated resonances
- still considering a pure target: one nuclide
- assign a weight to each resonance

$$w_i = \left(\frac{\Gamma_\gamma}{E_{res}^2} \cdot \frac{g\Gamma_n}{\Gamma} \right)_i$$

where

- Γ_n is the neutron scattering width
- g is the statistical factor, (2J + 1)/(2(2I + 1))
- J is the spin of the resonance state
- I is the spin of the target nucleus
- form an average self-shielding factor from all resonances of interest

$$\langle G_{res} \rangle = \frac{\sum w_i G_{res}(z_i)}{\sum w_i}$$

Model development, third step

- extend $\langle G_{res} \rangle$ to form the average for resonances of a mixture of nuclides
- assume the resonances of different nuclides do not overlap significantly

- make $\langle G_{res} \rangle$ energy dependent by taking averages separately for each energy bin used for the group-wise cross-sections
- use Fröhner's simple expression for the peak cross-section of each resonance (not available from the GENDF data)

Application of the model in FISPACT-II

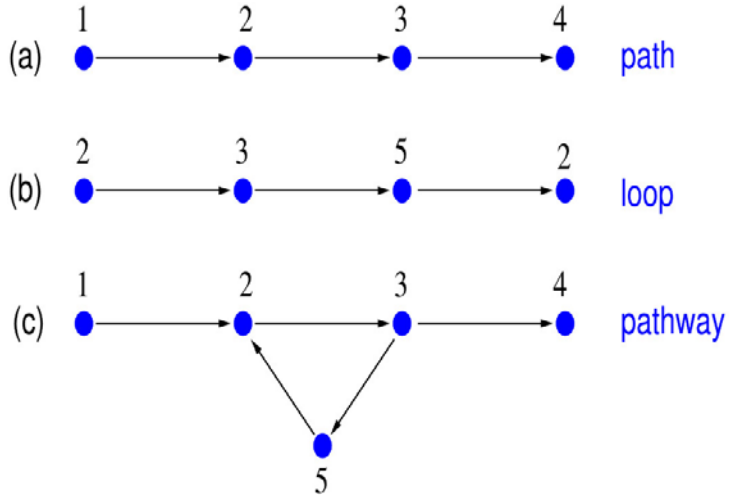
- universal curve model provides an alternative to probability table self shielding
- use $\langle G_{res} \rangle(E)$ to scale down energy-dependent cross-sections before cross-section collapse
- $\langle G_{res} \rangle(E)$ reduces the neutron flux, so apply it to all cross-sections
- target geometry specified with

  SSFGEOMETRY type $length_1$ <$length_2$ >
- use resonances from mixture specified with **SSFFUEL** or **SSFMASS**
- PRINTLIB 6 now generates a table of all cross-sections with $\langle G_{res} \rangle$ reduction factors

Extended pathways search

Pathways

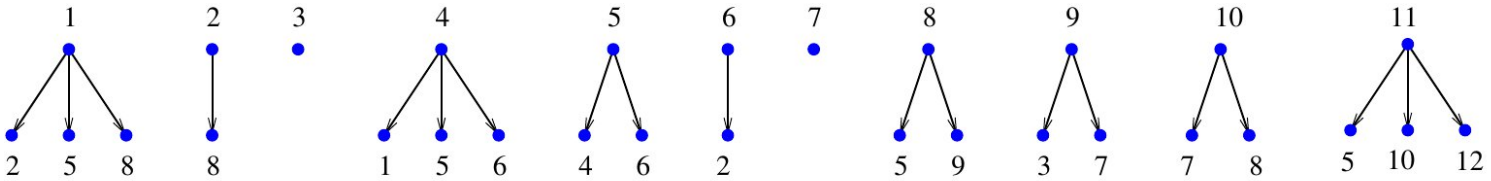
- Pathway = path + loop(s)
- Finds reaction/decay chains
- Identifies important
  - Nuclides
  - Reactions
  - Decays



- Used for uncertainty and sensitivity calculations

- Simple previous approach could fail through combinatorial explosion

Pathways – single visit tree

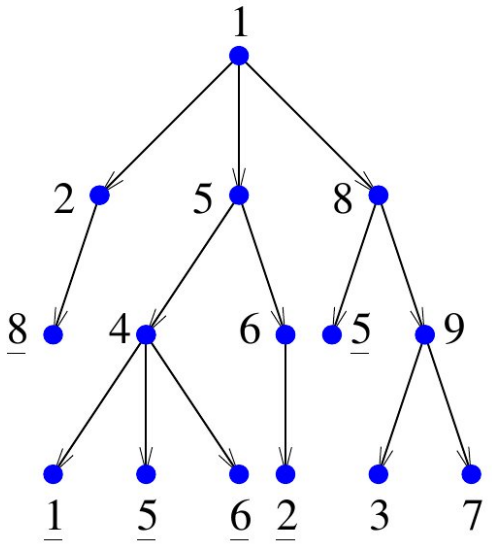


Adjacency lists

- tree search gives reduced p-d set
- pruning controlled using
  - path_floor
  - loop_floor
  - max_depth

- TENDL library
  - 3873 nuclides, ~240000 reactions
  - ~160,000 p-d pairs (57/nuclide)
  - single visit breadth-first search BFS

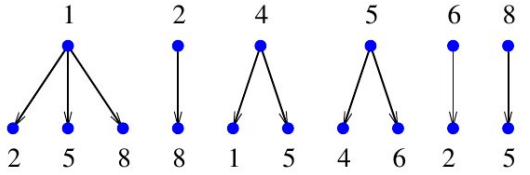
  typically < 50 p-d (parent-daughter)



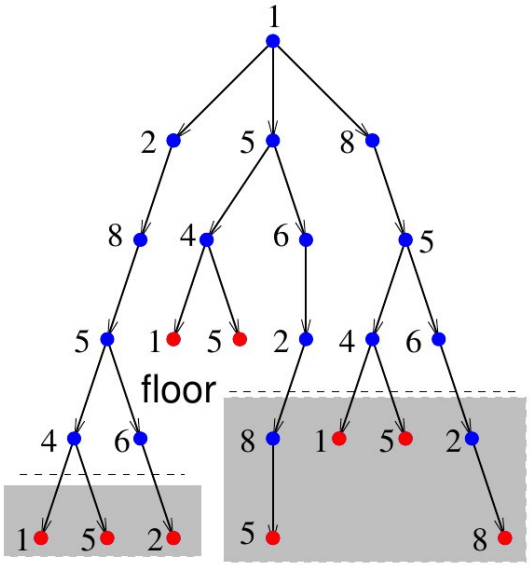
Single visit BFS tree for nuclide 1

Pathways

- build full tree for reduced p-d set
- leaf node if
  - repeat nuclide (loop)
  - path inventory below path floor
  - path depth greater than max depth
- combine paths and loops
- control keywords
  - `UNCERTAINTY (path_floor, loop_floor, max_depth)`
  - `SORTDOMINANT (topxx)`
  - `TOLERANCE (absolutetol_path, relativetol_path)`
  - `ZERO`
  - `LOOKAHEAD`
  - `PATHRESET`



nuclide 1 to 4 path edges



full tree with pruning

paths: 154 1854 12854
loops: 1541 545

Standard pathways calculation

- Initiated by `ZERO` keyword
- Combined `topxx` from dominant lists
- May miss late cooling time dominant nuclides

- Some typical ‘fixes’ to increase the depth of the simulation for more demanding simulations:
  - Reduce `path_floor` (prune fewer pathways)
  - Increase `topxx` (more dominant nuclides)
  - Use `LOOKAHEAD` (finds dominant nuclides at late times)
  - Use `PATHRESET` (re-calculates pathways at requested time)

Pathways with LOOKAHEAD

- LOOKAHEAD causes two-pass cooling:

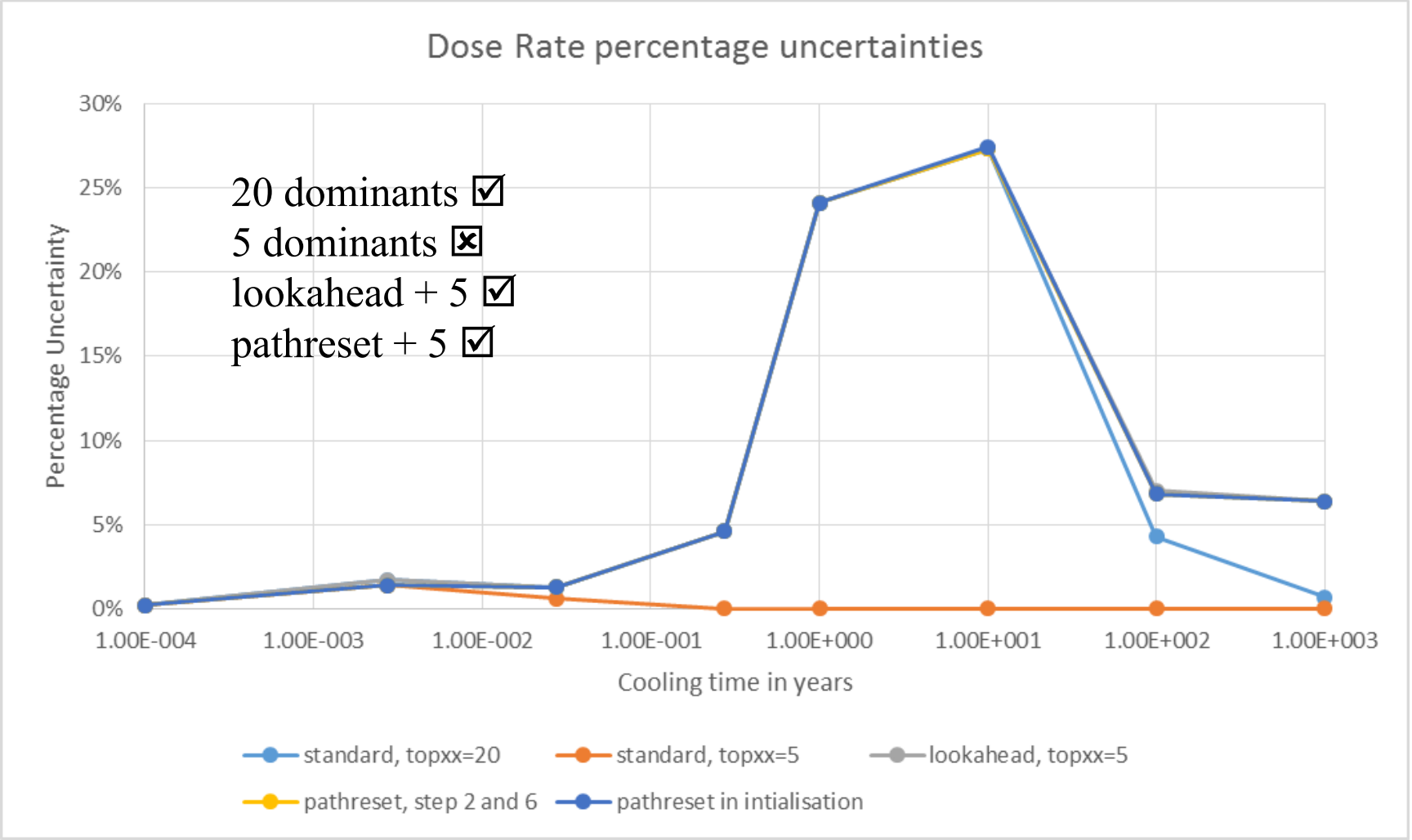
- at ZERO, integrate cooling steps to get late time dominant nuclides
- merge additional dominants with dominant list at ZERO
- use merged list in pathways calculation

Pathways with PATHRESET

- Save dominant list at ZERO, *ie* the end of irradiation
- PATHRESET in cooling phase:
  - At PATHRESET keyword, check for new dominant nuclides
  - If no new dominant nuclides, do nothing
  - If found, redo pathways calculation with current dominant list
- PATHRESET in initialisation phase
  - Same as PATHRESET at all cooling steps

Example: dose rate for SS316

- standard cases show late cooling time underestimates uncertainty; 25% at 1-10 years cooling



Charged incident particles, high-energy and residuals

Projectile choice

- FISPACT-II can handle the incident nuclear data for five particles, which are selected using the `PROJECTILE` keyword
  - `PROJECTILE 1` neutrons (default if not stated)
  - `PROJECTILE 2` deuterons
  - `PROJECTILE 3` protons
  - `PROJECTILE 4` alphas
  - `PROJECTILE 5` gammas
- For neutrons, the 1102 group data are used (and any other should the user wishes too)
- For charged particles, the 162 group is used instead
  - Note that `GETXS 1 162` must be used as well

TENDL residual nuclide production

- Above 30 MeV, reaction channel uniqueness breaks down as a functional description within ENDF-6
  - Too many reactions for < 200 mt values
  - Many reactions give equivalent products
  - Only total residual production tends to have experimental data
- At 30 MeV TENDL changes from specific-mt descriptions to mt=5 mf=10 yield data
- These include summation over all reaction channels and condense the data into yield x cross-section for production of each residual nuclide

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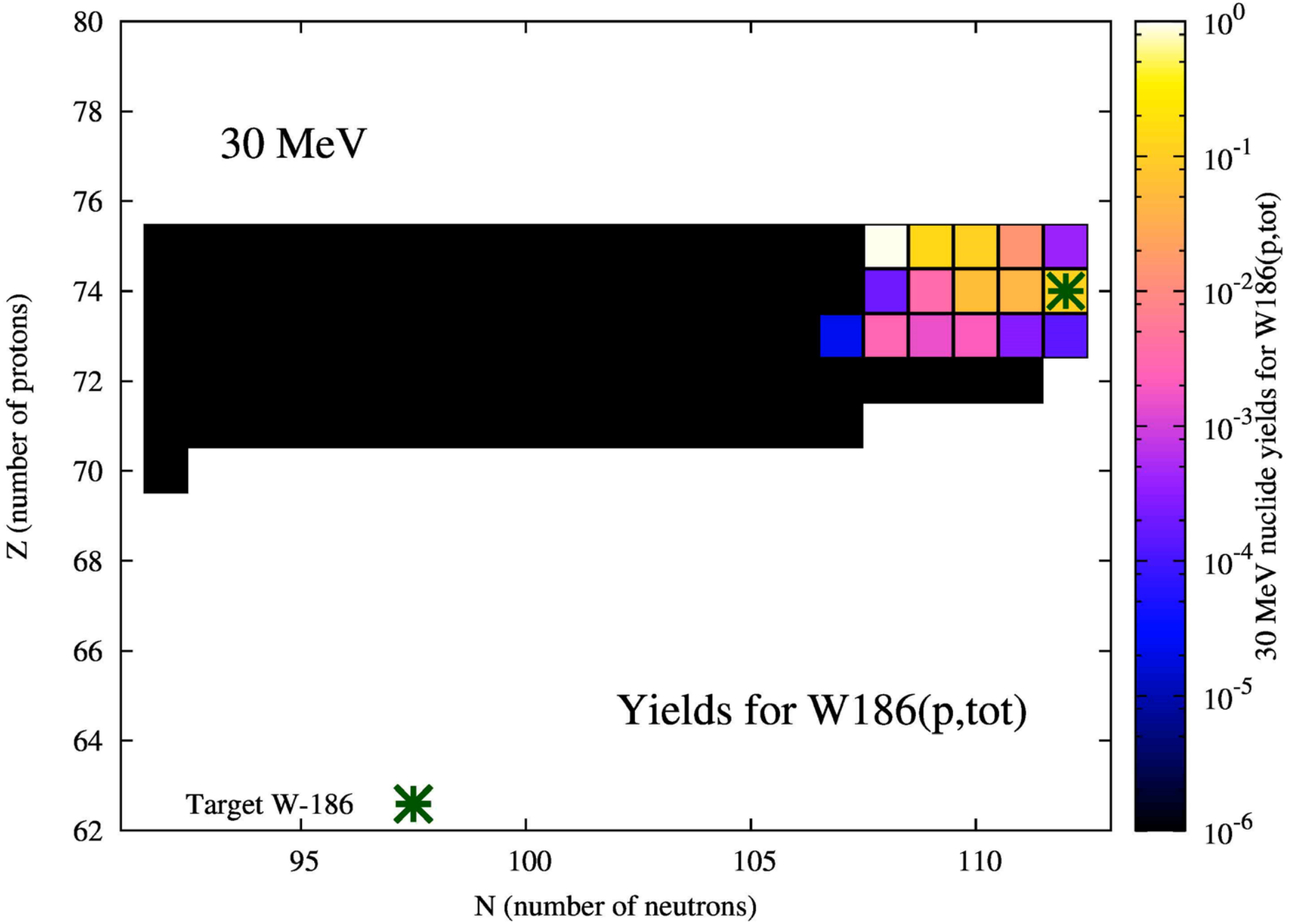
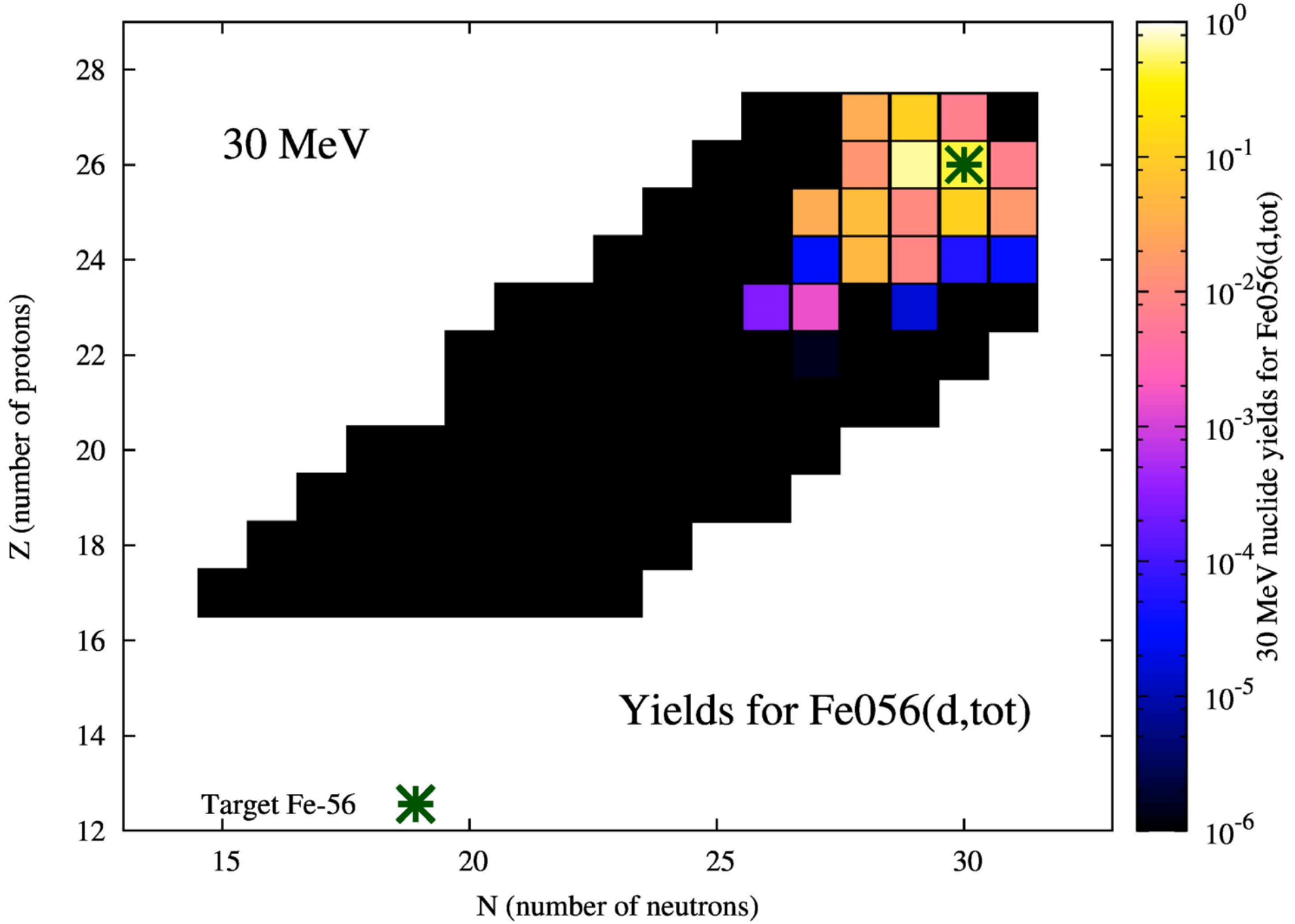
W-186 proton irradiation



UK Atomic Energy Authority

F-56 deuteron irradiation



Fission addition

- TENDL contains additional knowledge of fission cross sections which are stored and read by FISPACT-II above 30 MeV
- These exist for neutron-induced reactions as well as proton, deuteron, alpha, gamma…
- The remaining data required for these are fission yields. While these are not supplied in the standard FISPACT-II distribution, approximate files can be generated by any suitable code (*eg* GEF)
  - FISPACT-II can read these (in ENDF6 format) within the same *fy_endf* directory irrespective of incident particle

FISPACT-II web site

- http://fispact.ukaea.uk/

UK Atomic Energy Authority

FISPACT-II

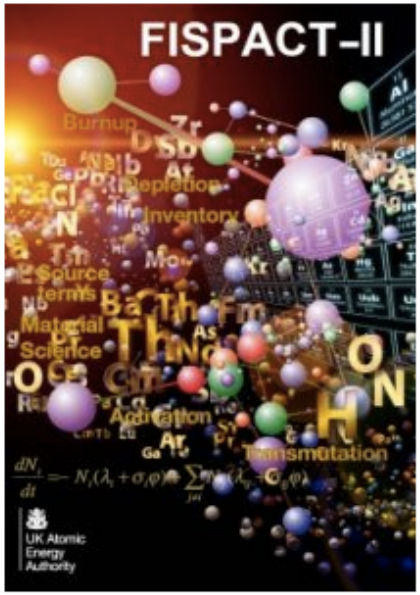
Overview | Methods » | Documentation » | Validation » | Nuclear data » | Links » | Contact | English »

Overview

FISPACT-II is an enhanced multiphysics, inventory and source-term code system providing a wide variety of advanced, predictive, spectral and temporal simulation methods employing the most up-to-date and complete nuclear data forms for both neutron and charged-particle interactions.

FISPACT-II has been developed and is maintained by the United Kingdom Atomic Energy Authority at Culham. As a comprehensive, modern object-oriented Fortran code, FISPACT-II fully processes all ENDF-6 nuclear data including the complete TENDL data with full covariances files. This extends the physics up to GeV energy with all channels and incident/emitted particles. Code features include self-shielding factors, broad temperature dependence, thin/thick target yields, robust pathway analysis, Monte-Carlo sensitivity and uncertainty quantification and propagation using full covariance data.

The latest generation of processing codes PREPRO, NJOY and CALENDF are used to provide the user with the most sophisticated incident-particle nuclear data from the TENDL-2015, ENDF/B.VII.1, JENDL-4.0, CENDL-3.1 and JEFF-3.2 international libraries, which are complemented with the latest decay and fission yield data, including the most recent GEFY-5.2 libraries. The maturity of modern, technological nuclear data including TENDL and GEF provides truly comprehensive data for all simulation requirements. The result is a multiphysics platform that can accommodate the needs of all nuclear applications including: activation, transmutation, depletion, burn-up, decays, source definition, full inventories, dpa, kerma, primary damage (PKA) spectra, gas/radionuclide production and more.



FISPACT-II web site

ICTP Trieste Nuclear Data Workshop Oct 2-13 2017

The Joint ICTP-IAEA Workshop on the Evaluation of Nuclear Reaction Data for Applications will be held in Trieste, October 2-13 2017. There is no registration fee. The deadline for applications ...

Read More

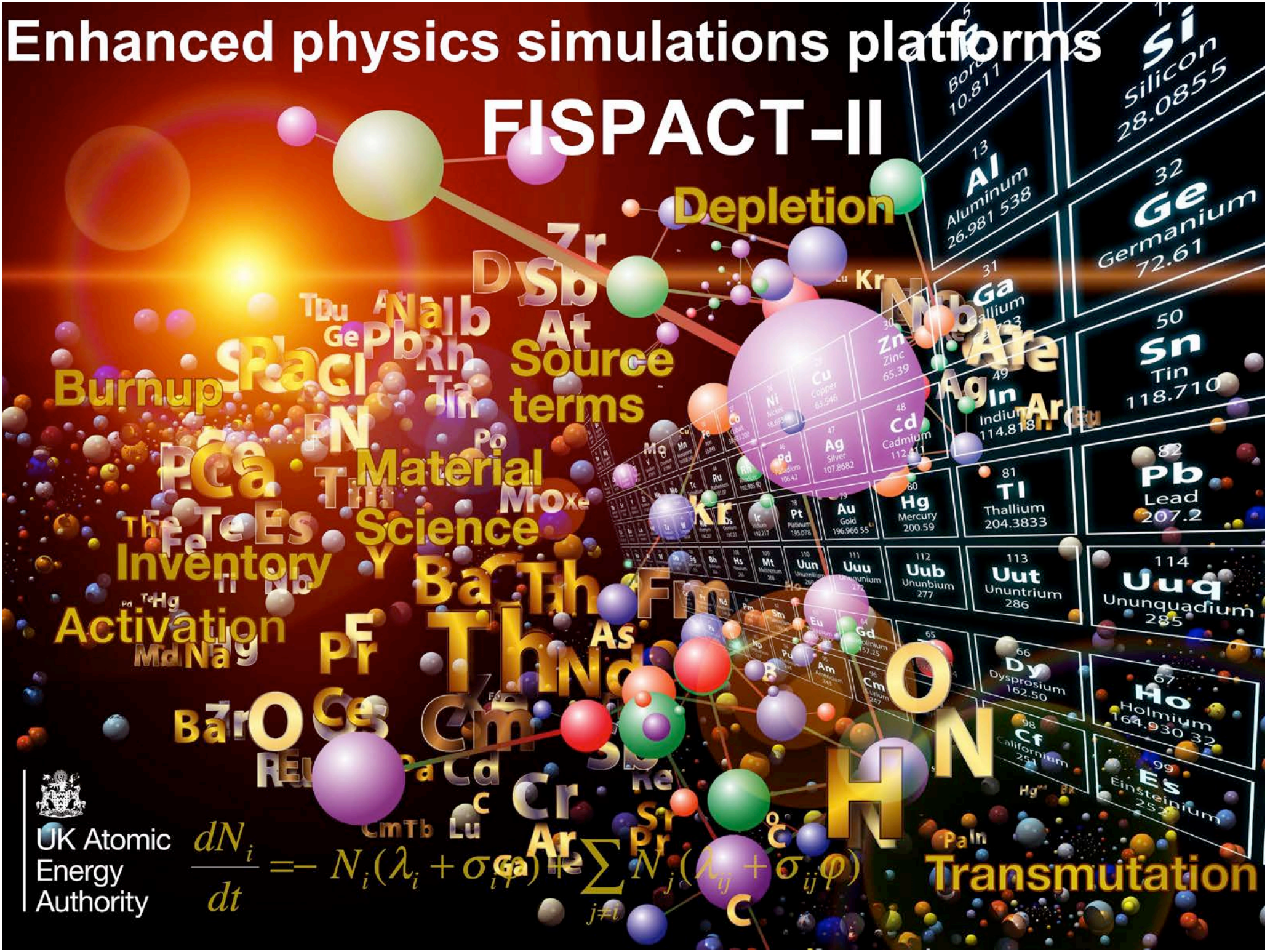
5th July 2017 / Michael Fleming / Nuclear Data, Training, Workshops

Workshop on TALYS/TENDL developments, 13-15 November 2017, Prague

FISPACT-II 3-20 available through OECD-NEA Data Bank

FISPACT-II 3-20-00 code release

FISPACT-II 3-00-00 available through ORNL RSICC


Enhanced physics simulations platforms
FISPACT-II
Depletion
Source terms
Material
Science
Inventory
Activation
Transmutation
Burnup
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$\frac{dN_i}{dt} = -N_i(\lambda_i + \sigma_i \varphi) + \sum_{j \neq i} N_j(\lambda_{ij} + \sigma_{ij}\varphi)$