Enhanced physics simulations platforms

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1. Nuclear data purpose and source

2. Present inadequacies of major code systems for fusion and advanced applications

3. Solutions with technological nuclear informatics

4. EASY-II: technological data with modern simulation

5. Status, validation and unique capabilities

6. Position for UKAEA moving forward
• Nuclear simulation codes (SERPENT, MCNP, FISPACT-II, etc.) do not contain all physics of particle interaction (cross section, angular/energy emitted spectra) but read from nuclear data tables

• Knowledge of nuclear interactions derived from careful and expensive experiments + sophisticated modelling

• Decades of effort has resulted in relatively reliable information for simulation of LWRs and other specific applications – using tiny fraction of nuclides/reactions

• Simulation of fusion reactors, advanced systems will require substantially greater library with much more detail than simple $\sigma(E)$
• Raw nuclear data files are pretty useless!

• Nuclear data processing is a necessity: to feed the many nuclear codes that require processed nuclear data forms

• These data are used by particle transport; MCNP, SERPENT and time-evolution/inventory codes such as FISPACT-II

• The physics of interaction probabilities, emitted spectra, decays/heat/activity, etc. are taken from nuclear data

• Processing bridges the gap between the physics and the simulation codes
Simulation in space, energy and time

**Boltzmann equation**
- transport
- time independent
- energy and spatial simulation
- primary response

**Bateman equation**
- inventory
- time dependent
- secondary response

**Nuclear Data**

**TENDL**
- EU

**Carousels**
- TRIPOLI
  - EU
- SERPENT
  - EU
- MCNP6
  - US

**API**

**FISPACT-II**
- EU

**Number densities** $(t_n)$
- Prompt spectra
- Reaction rates

**Number densities** $(t_n + \Delta t)$
- Secondary, decay spectra
- Irradiation conditions

**Application Program Interface**: interfaces to connect Boltzmann and Bateman solvers for non-linear $t$- and $T$-dependent transport
• Well-known nuclear data libraries (ENDF-US/JENDL-Japan/ JEFF-OECD) assembled over decades by hand: ‘evaluators’ added nuclides/reactions when it was deemed necessary

• Methodology strong where we know answers, but:
  - Relative to total set of nuclides/reactions, they are tiny
  - They change only when experiments explicitly show errors
  - They will not contain any more than a very small fraction of the nuclides/reactions needed for other applications

• Since many (or most) reactions important for advanced systems (particularly fusion) have little or no experimental data, legacy data **can not be used for these systems**
• Since legacy libraries cannot satisfy needs for fusion/adv. systems, an alternative is necessary

• TALYS code suite (NRG-Petten) uses various physical models (theoretical and semi-empirical) to generate TENDL data library

• TENDL library covers complete nuclide/reaction set, preventing under-estimation due to missing data

• A precursor of TALYS was used to generate EAF library
TALYS code scheme

**Input:**
- Keywords, e.g.: projectile n element fe mass 56 energy 14.

**Optional loops**
- Incident energies
- Natural isotopes

**Nucl. Structure:**
- Abundancies
- Discrete levels
- Deformations
- Masses
- Level density par.
- Resonance par.
- Fission barrier par.
- Thermal XS
- Microscopic LD
- Precession shapes

**Optical Model:**
- Phenomenology local / global

**Direct reaction:**
- Spherical OM
- DWBA
- Rotational CC
- Vibrational CC
- Giant resonances
- Weak-coupling

**Preequilibrium:**
- Exciton model
- 2-component
- p-h LD phenom.
- surface effects
- Kalbach systematics
- angular distribution
- cluster emission
- \( \gamma \)-ray emission

**Compound:**
- Width fluctuations
  - Moldauer
  - GOE triple integr.
  - HRTW
- Hauser–Feshbach
- Fission competition
  - isotopic yields
- All flux depleted
- Exclusive channels
- Recoils

**Multiple emission:**
- Exciton (any order)
- Hauser–Feshbach
- Fission competition
- Isotopic yields
- \( \gamma \)-ray cascade

**Output:**
- File ‘output’ defined by keywords
- Dedicated files with spectra, ...

**ENDF:**
- Transport libs
- Activation libs
Total Monte Carlo = TMC

Loop over parameters: Total Monte Carlo

Experimental nuclear physics

- EXFOR Database
- Nuclear model input parameter database
- Theoretical nuclear physics

Nuclear model software

- TARES resonances
- TAFIS nubar
- TANES fis. neutrons
- TALYS fast energies

Nuclear data library

- TEFAL ENDF fmt
- Older ENDF library

Testing and processing

- ENDF library
- NJOY
- PREPRO
- CALENDF
- Processed library

Processed library

- BNL checking codes

Neutronics, depletion Reactor physics

- MCNP
- SERPENT
- DRAGON
- FISPACT

Criticality (k-eff)
- Reactivity coeff. (Doppler, void)
- Reactivity swing
- Inventory
- Radiotoxicity
- Shielding spectra

SAVE INPUT FILES
• EAF relied upon legacy evaluation methodology

• EAF2007/10 were the best activation libraries until TENDL began (2008), and have been quickly overtaken

• Complete TENDL library generated each year since 2008, with 2014 completely validated and demonstrably superior

• New functionalities of FISPACT-II, Spectra-ER and MCNP6 are exclusively compatible with TENDL (due to EAF format and physics insufficiencies)

http://www.ccfe.ac.uk/easyii_validation.aspx
European Activation SYstem

EASY–II

Astrophysics

Depletion

Fission

Criticality

At

Source terms

Material Science

Fusion Burnup

Inventory

Activation

Pile

Reactor

Medical

Transmutation

\[
\frac{dN_i}{dt} = -N_i(\lambda_i + \sigma_{ip}) + \sum_{j=1} N_j(\lambda_{ij} + \sigma_{ij})
\]
EASY-II roadmap

1. FISPACT-2007+ & EAF-2010 in EAF format processed by SAFEPAQ-II ✓ 08/2010
2. FISPACT-II(11) & EAF-2010 in EAF format processed by SAFEPAQ-II ✓ 01/2011
3. FISPACT-II(11) & EAF-2010 + CAENDF PT’s ssf method, ENDF’s format and processing framework ✓ 09/2011
4. EASY-II(12) = FISPACT-II(12) & EAF’s and TENDL-2011 ENDF’s libraries processed by NJOY, PREPRO & CALENDF ✓ 03/2012
5. EASY-II(13) = FISPACT-II & EAF’s and TENDL’s V&V libraries processed by NJOY, PREPRO & CALENDF ✓ 06/2013
6. EASY-II(14) = FISPACT-II & EAF’s, TENDL’s, ENDF’s libraries, some automated V&V processes ✓ 07/2014
7. EASY-II(15) = FISPACT-II & TENDL’s, ENDF’s libraries, all automated V&V processes 08/2015

Vigilant, thorough V&V stepped approach
### FISPACT-II versus FISPACT-2007

<table>
<thead>
<tr>
<th>Feature</th>
<th>FISPACT-II</th>
<th>FISPACT-2007</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Solver</strong></td>
<td>Numerical - LSODES 2003</td>
<td>Numerical - EXTRA 1976</td>
</tr>
<tr>
<td><strong>Incident particles</strong></td>
<td>$\alpha, \gamma, d, p, n$ (5)</td>
<td>$d, p, n$ (3)</td>
</tr>
<tr>
<td><strong>ENDF’s libraries: TENDL-2014, ENDF/B-VII.1, JEFF-3.2, JENDL-4.0</strong></td>
<td>✔ XS data (2632 targets) ✔ Decay data (3873 isotopes)</td>
<td>✗</td>
</tr>
<tr>
<td><strong>Dpa, Kerma, Gas prod., radionuclide yields</strong></td>
<td>✔</td>
<td>✗ (Gas production)</td>
</tr>
<tr>
<td><strong>Uncertainty</strong></td>
<td>✔ Variance-covariance</td>
<td>✔ 1 to 3 broad groups</td>
</tr>
<tr>
<td><strong>Temperature</strong></td>
<td>0, 294, 600, 900 K,…30 KeV</td>
<td>294 K</td>
</tr>
<tr>
<td><strong>Self-shielding</strong></td>
<td>✔ Resolved and Unresolved Resonance Range</td>
<td>✗ infinitely dilute cross section</td>
</tr>
<tr>
<td><strong>Energy range</strong></td>
<td>$1.0 \times 10^{-5}$ eV – 200 MeV</td>
<td>$1.0 \times 10^{-5}$ eV - 55 MeV</td>
</tr>
<tr>
<td><strong>Sensitivity</strong></td>
<td>✔ Monte Carlo</td>
<td>✔ sensitivity coefficient</td>
</tr>
<tr>
<td><strong>Pathways</strong></td>
<td>✔ multi steps</td>
<td>✔ single step</td>
</tr>
<tr>
<td><strong>Thin, thick targets yields</strong></td>
<td>✔</td>
<td>✗</td>
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</table>
EASY-II development

**Enhanced Physics**
- Prompt, delayed and decay source terms for neutron, charge particles and residuals:
  - spontaneous fissions, all fissions (GEF)
  - \((\alpha,n), (\gamma,n), (p,n), (d,n),\ldots\)
  - Antineutrino from beta decay
  - Continuous, discrete spectrum
- Uncertainty quantification and propagation

**Coding improvements**
- Multiple projectiles irradiation scenario
- Multi-threading, parallelism
- API Application Programming Interface

**Verification and Validation**
- Automated Verification and Validation processes
- Nuclear data visualisation tools
Validation of FISPACT-II and its nuclear data libraries through multi-faceted effort including variety of code applications: MCF, ICF, advanced fission, high energy and accelerator, medical, isotope production, earth explorations, astrophysics.

Each of the following completed or will be by mid-2015:
- Detailed analysis of fusion total heat measurements done at JAEA/FNS
- Validation of all existing integro-differential activation experiments
- Simulation of complete set of material properties under irradiation
- In-depth simulations of fission decay heat with break-down of nFY/decay/spectroscopic analysis
- Massive validation against library of integral data from integral resonance, astrophysics and fission sources

No comparable system has undergone equivalent V&V
random-walk

FNS-00 5 Min. Irradiation - Ni

<table>
<thead>
<tr>
<th>Product</th>
<th>Pathways</th>
<th>$T_{1/2}$</th>
<th>Path %</th>
<th>E/C</th>
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<tr>
<td>$^{62}\text{Co}$</td>
<td>$^{62}\text{Ni}(n,p)^{62}\text{Co}$</td>
<td>1.5m</td>
<td>99.8</td>
<td>0.90</td>
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<tr>
<td>$^{62m}\text{Co}$</td>
<td>$^{62}\text{Ni}(n,p)^{62m}\text{Co}$</td>
<td>13.9m</td>
<td>100.0</td>
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Heat Output [$\mu$W/kg] vs. Time after irradiation [minutes]
Time: 0.00 seconds
Total Decay Heat (kW/kg): 0.0

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<tr>
<th>Z</th>
<th>N</th>
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</tbody>
</table>

FNS-00 5 Min. Irradiation - SS316

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

M.R. Gilbert & J.-Ch. Sublet CCFE-R(14)21 JAEA FNS Decay heat validation
M. R. Gilbert et al., "Inventory Visualisation techniques" Nucl. Sci. Eng (2014)
V&V: Integro-differential validation

- Inclusion of meta-stables substantially improves simulation accuracy

Y90m measured

$\text{Nb93}(n,\alpha)\text{Y90m}$

$T_{1/2} = 3.1\text{h}$
C/E distributions for integral measurements

Top: TENDL-2014 outperforms EAF10 – the latter was specifically tuned to these!

Bottom: all legacy libraries (ENDF, JENDL, JEFF shown) miss tremendous number of reactions entirely

*TENDL will become standard*
• Simulation of complex fission burst decay experiments – Pu241 thermal ‘pulses’ above, with reconstruction of irradiation conditions
V&V: Decay heat following a thermal pulse

- Comparison between libraries for U235 total and gamma contributions to decay heat - note gamma deficiency

- ENDFB/JENDL include TAGS to correct $\gamma$

- FISPACT-II can track all nuclides for in-depth study

- Contribution to DH needs for $\nu + TAGS$
Probing decay data and nFY discrepancies

U235 Dominant Gamma Heat Nuclides at 10s
• Non-threshold: therm, MACS, IR, etc

• Most standard, but MACS for plasma, not 0K

• Some nucleo-synthesis reactions have little RRR -> problem MACS
• Statistical reconstruction allows thinned astrophysical values based on level parameters, which can be at 30keV
MACS example: Er166, TENDL vs Legacy

- MACS as \( f(kT) \)
- Inter & maxwav
- No CAL
- Data are KADoNiS
- Decent agreement >30keV
• PKAs in Fe under DEMO conditions:

- Primary knock-on atom (PKA) evaluations using TENDL-2014 and Spectra-er
- Necessary as input into materials modelling of radiation damage creation and evolution
• Ability to assemble, re-evaluate all types of nuclear data

• Ability to generate TENDL evaluated files with T6: TALYS, TEFAL, TANES, TAFIS, TARES, TASMAN

• Ability to creates rich multifaceted data forms through smart processing steps relying on PREPRO-2015, CALENDF-2010, NJOY-2012 and Spectra-ER

• Ability to automatize all processes

• From cradle to grave
Closing the technological loop

• The Total Monte Carlo (TMC) methodology uses direct feedback from simulation to physical inputs = TENDL

• TMC provides truly remarkable uncertainty analysis based upon simulation outputs – where legacy provides little/none

• TMC is as good as the simulation capability. The marriage of TENDL with simulation code provides the most robust methodology

By bringing the disjoint nuclear data links, from evaluation to application, into a technologically-driven closed system we can provide complete, robust data superior to any legacy system
Where we are now

• Technological TENDL-14 has surpassed evaluated EAF, routinely beats legacy libraries + adds new capabilities

• V&V results demonstrate strengths of EASY-II + TENDL – internally and to all fusion/fission collaborators

• Only a few laboratory have ability, will to integrate complete technological loop – from data construction to validation

• Modern simulation (fusion, advanced systems & security…) cannot occur without these developments (although non-physical calculations may)
To maintain the dominance, we must develop the tools which will be requested and required by the R&D community:

- FISPACT-II & MCNP6 (SERPENT2 ?) API (and general transport codes)
- Advanced data analysis and visualisation tools
- Multi- and sequential charged particle simulation
- Particle source terms (in collaboration with LANL)
- Code optimisation collapse/solver (demonstrated)

Further develop tools for use by the UKAEA and its partners to secure variety of funding streams
• UK Atomic Energy Authority (3 professional man years)
  ▪ Integrate TALYS code suite with processing and simulation codes to revolutionise nuclear data for advanced applications
  ▪ Develop FISPACT-II for advanced-system-critical capabilities

• Engage with UK NNL, R&R and NPL, the NDA

• Liaise with Cambridge University

• Collaborate with NRG, LANL, CEA and VTT?
21st century observables for nuclear sciences and technology: stockpile, fuel cycle stewardship, source terms, materials characterization and life cycle management for all application:

- Magnetic and inertial confinement fusion
- Advanced Fission Gen IV and beyond
- Advanced energy and fuel systems
- High energy and accelerator physics
- Medical applications, isotope production
- Earth exploration, Astrophysics
- Homeland security