UKAEA work with TALYS/TENDL and FISPACT-II

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

13 November 2017

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Agenda

Background

Integral fusion/accelerator

- Historical results
- TENDL-2017

Maxwellian-averaged data

- Processing/temperatures
- Temperature-dependent results

Upcoming developments

- FISPACT-II
- 'High'-energy data

Conclusions

TENDL V&V
Background

- Compared with other ENDF-6 nuclear data libraries, TENDL provides a *massive* amount of data
- (Bi-)annual library generation and release is much faster-paced than alternatives

- The combination of these two requires a validation process that is as complete and fast-paced as the TENDL generation process (or part of the generation)

UKAEA validation processes
Background

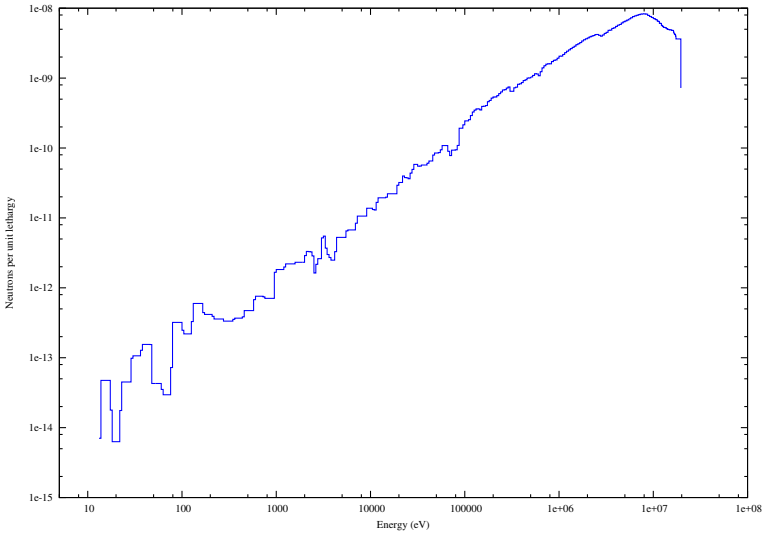
- The UKAEA has performed previous V&V for TENDL-2014 data, covering a range of integral measurements in fusion/accelerator systems, decay heat simulations, MACS and statistical checks
- `http://fispact.ukaea.uk/documentation-2/reports`

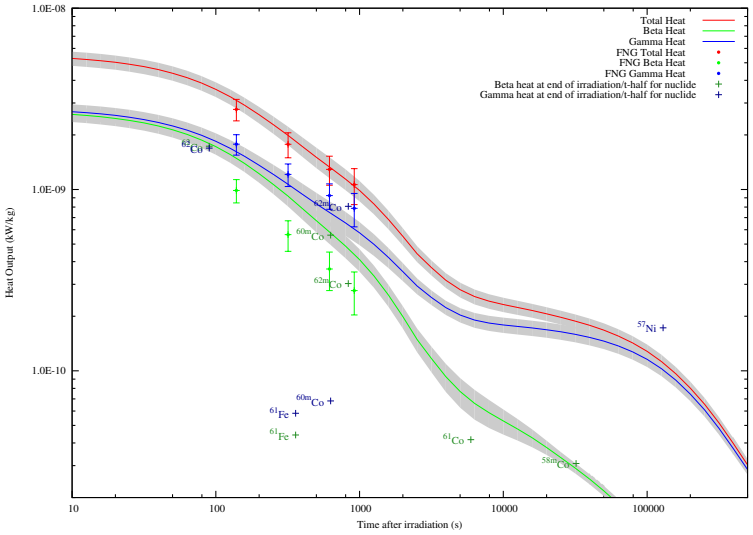
- See the presentations of Jean-Christophe Sublet and Arjan Koning for more information

Calculation methods

Updated validation processes

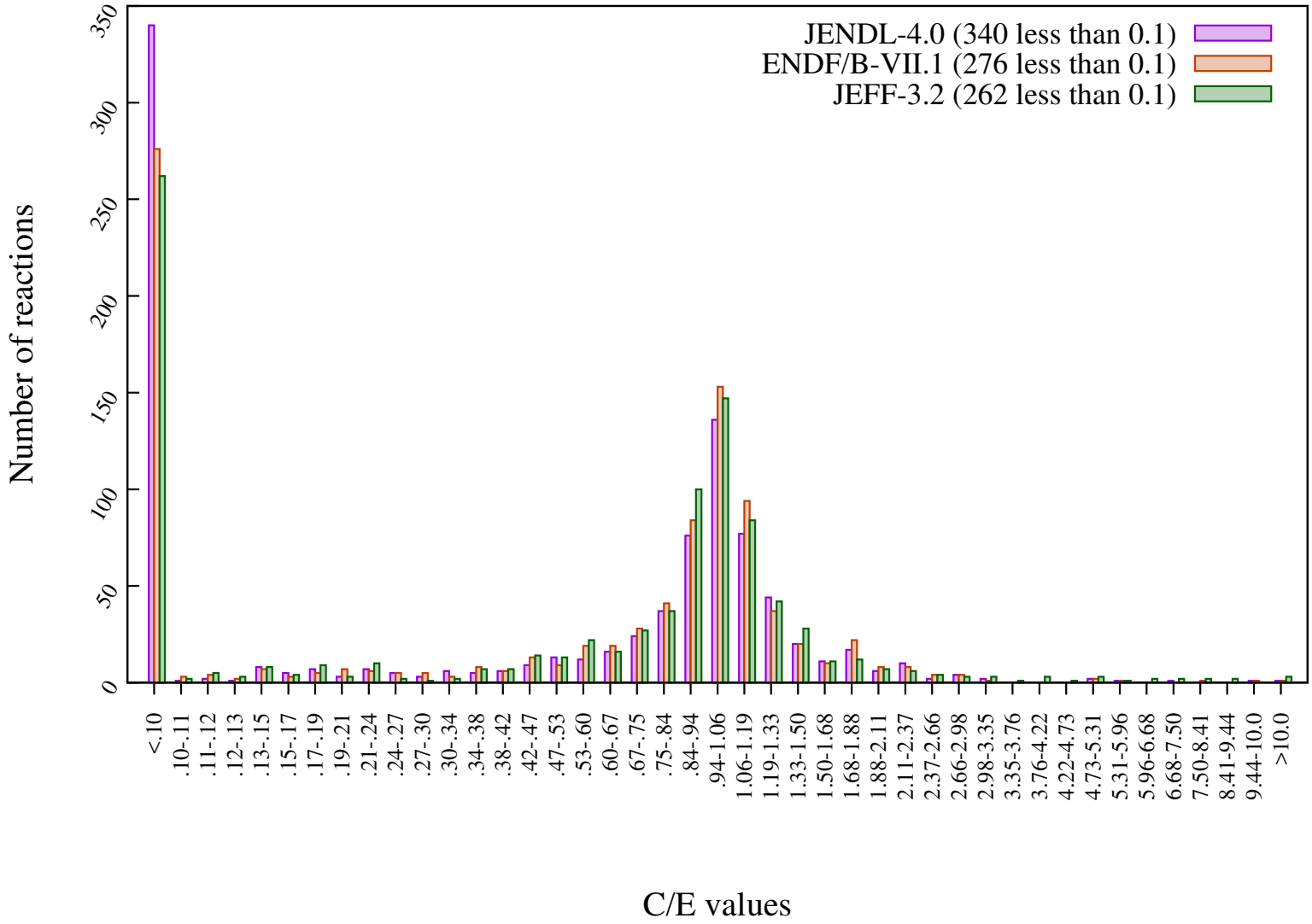
- Set of spectrum-averaged (integral) cross sections used with inventory calculations in FISPACT-II and compared with experiment
- New TENDL-2017 files are available for non-neutron reactions and a select few for neutron testing





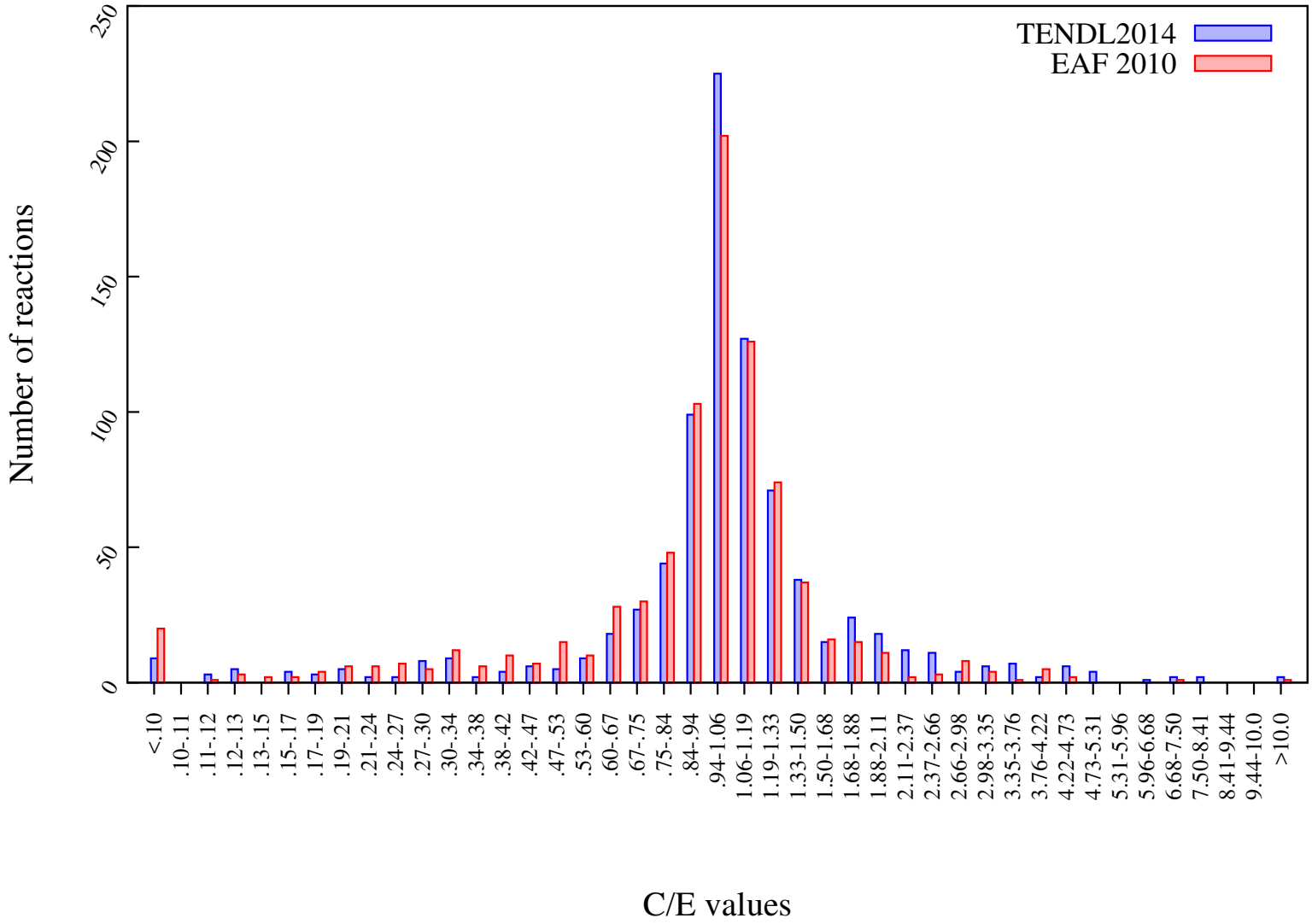
Historical results

Integral fusion/accelerator



Historical results

Integral fusion/accelerator

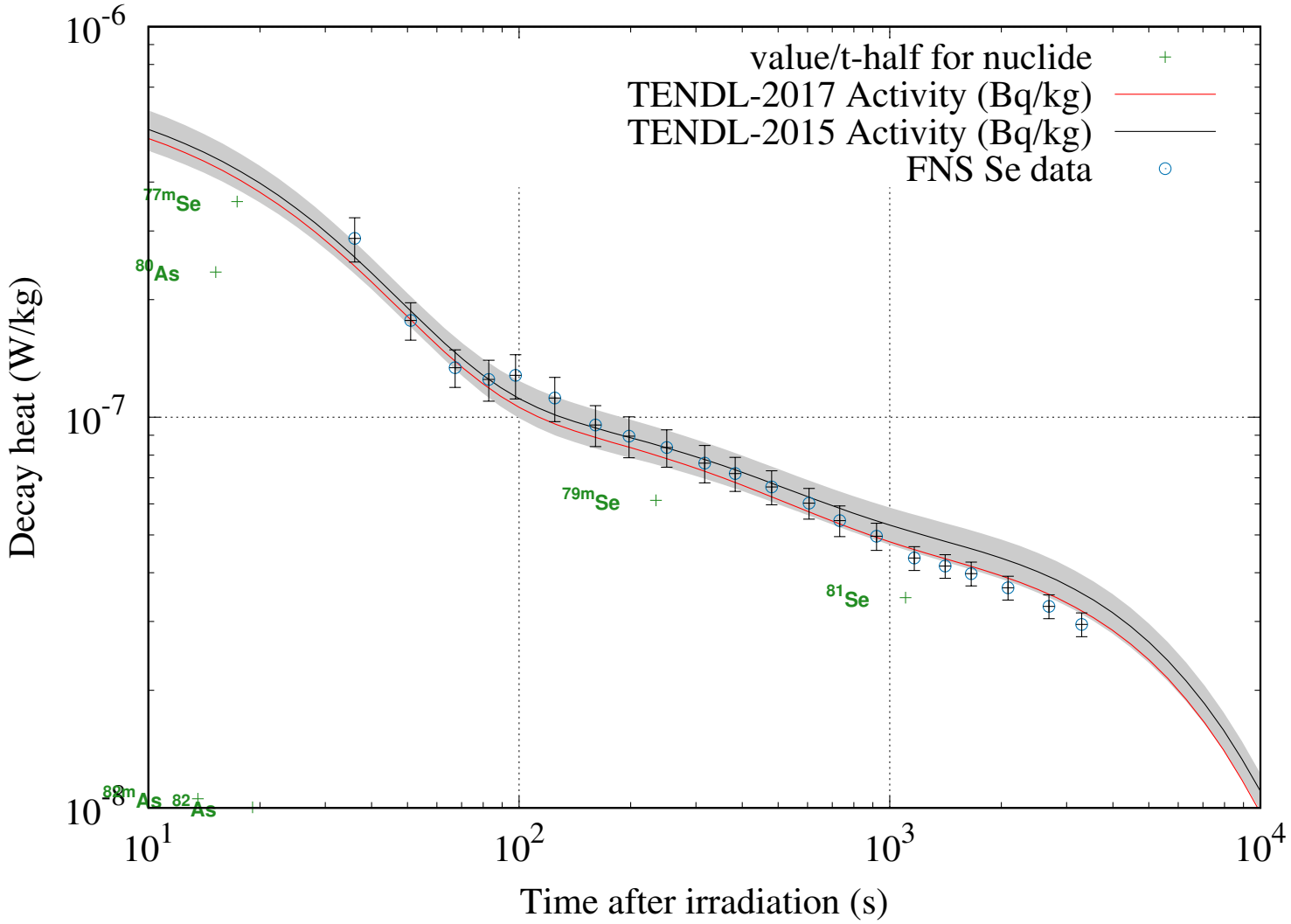


Overview
TENDL-2017

- Integral measurements cover some 158 target nuclides, including all isotopes
- Dominant measurements only consider certain reaction channels
- TENDL-2014/15 performance for 'high-quality' integral experiments, notably FNS decay heat, was already very good!
- Hunt for improvement is quite difficult!
- **See work (and presentation) of Natalia Dzysiuk** for improvements in the 'best' TALYS parameters

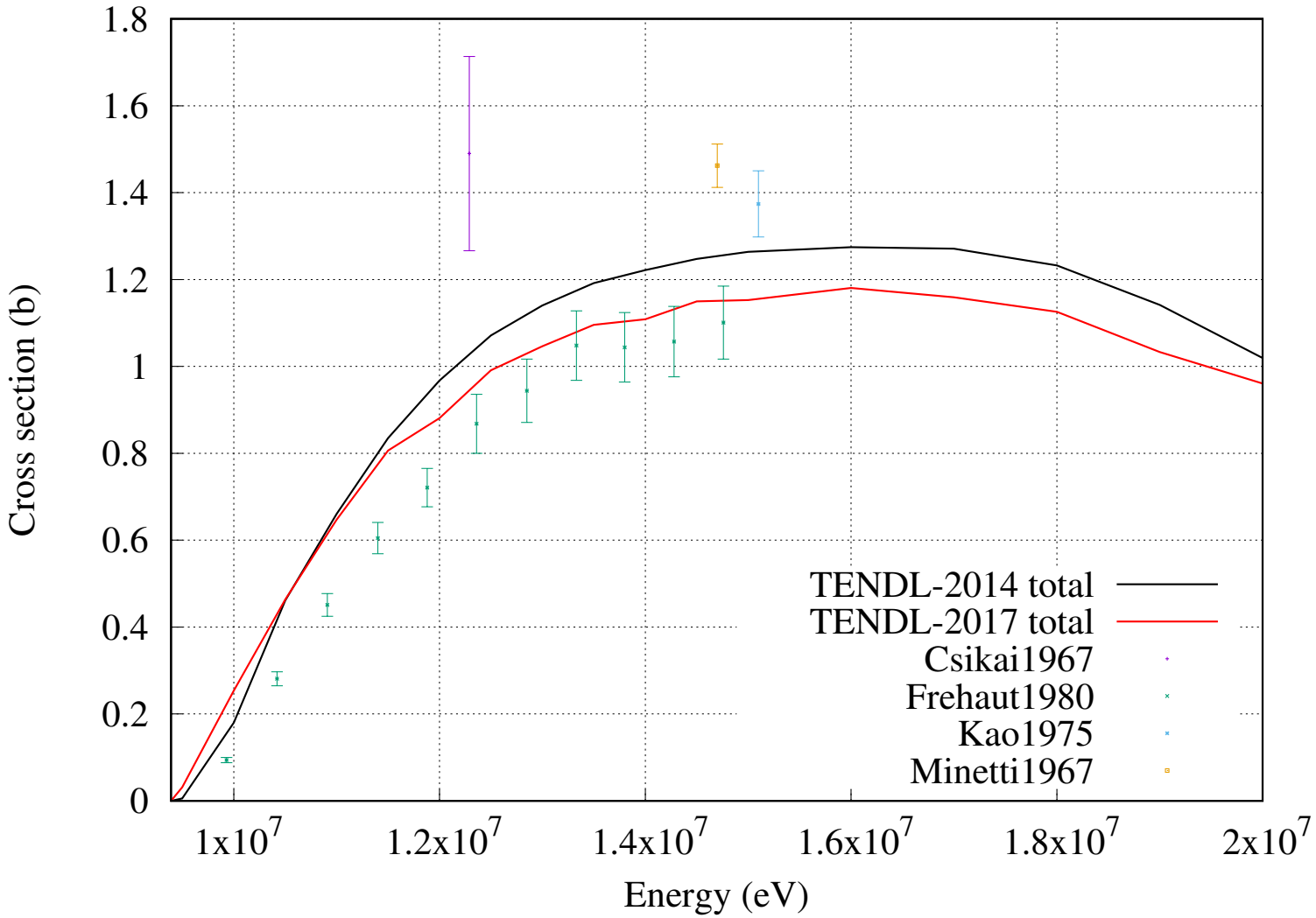
Example results - Se FNS

TENDL-2017



Example results - Se82(n,2n)

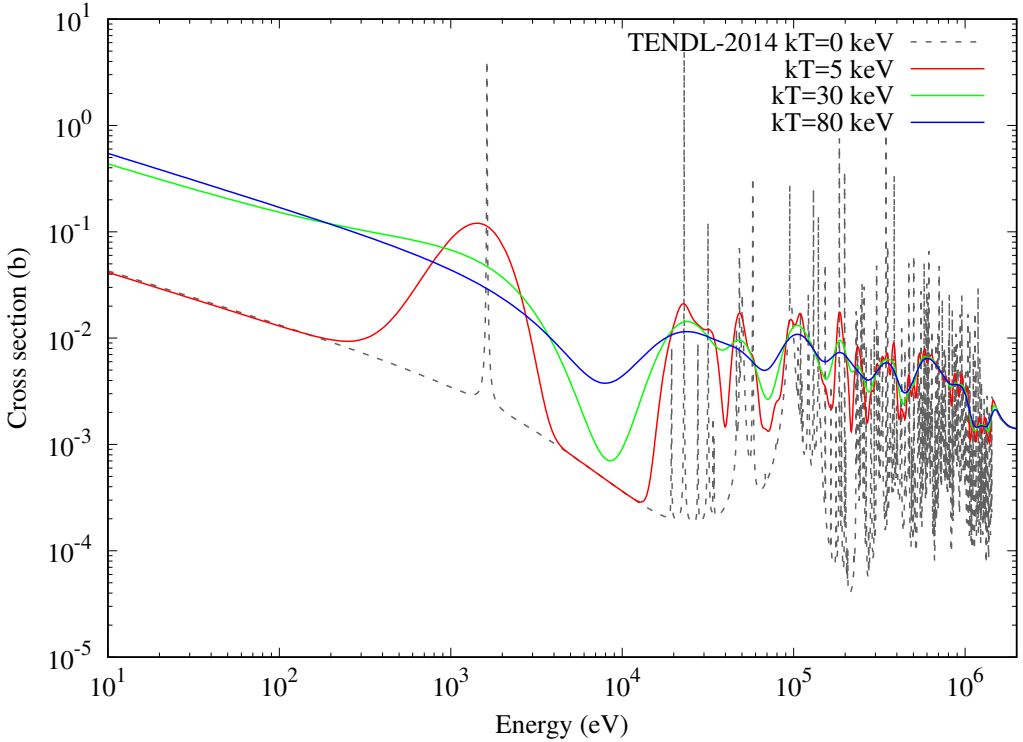
TENDL-2017



Processing/temperatures

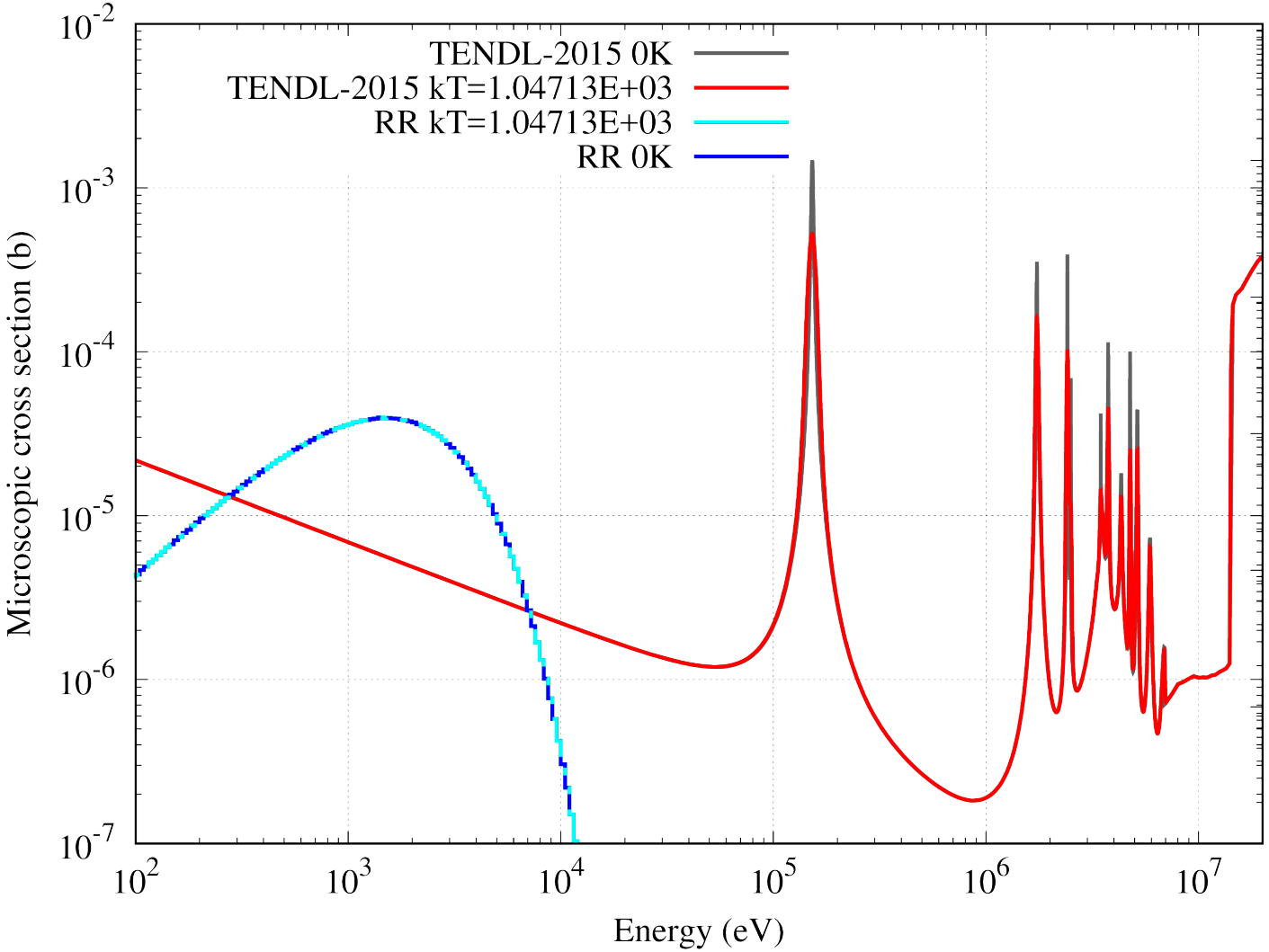
Maxwellian-averaged data

- For MACS integral cross sections, the target is at keV energies, requiring resonance broadening treatment
- Integral of Maxwellian neutron with broadened data



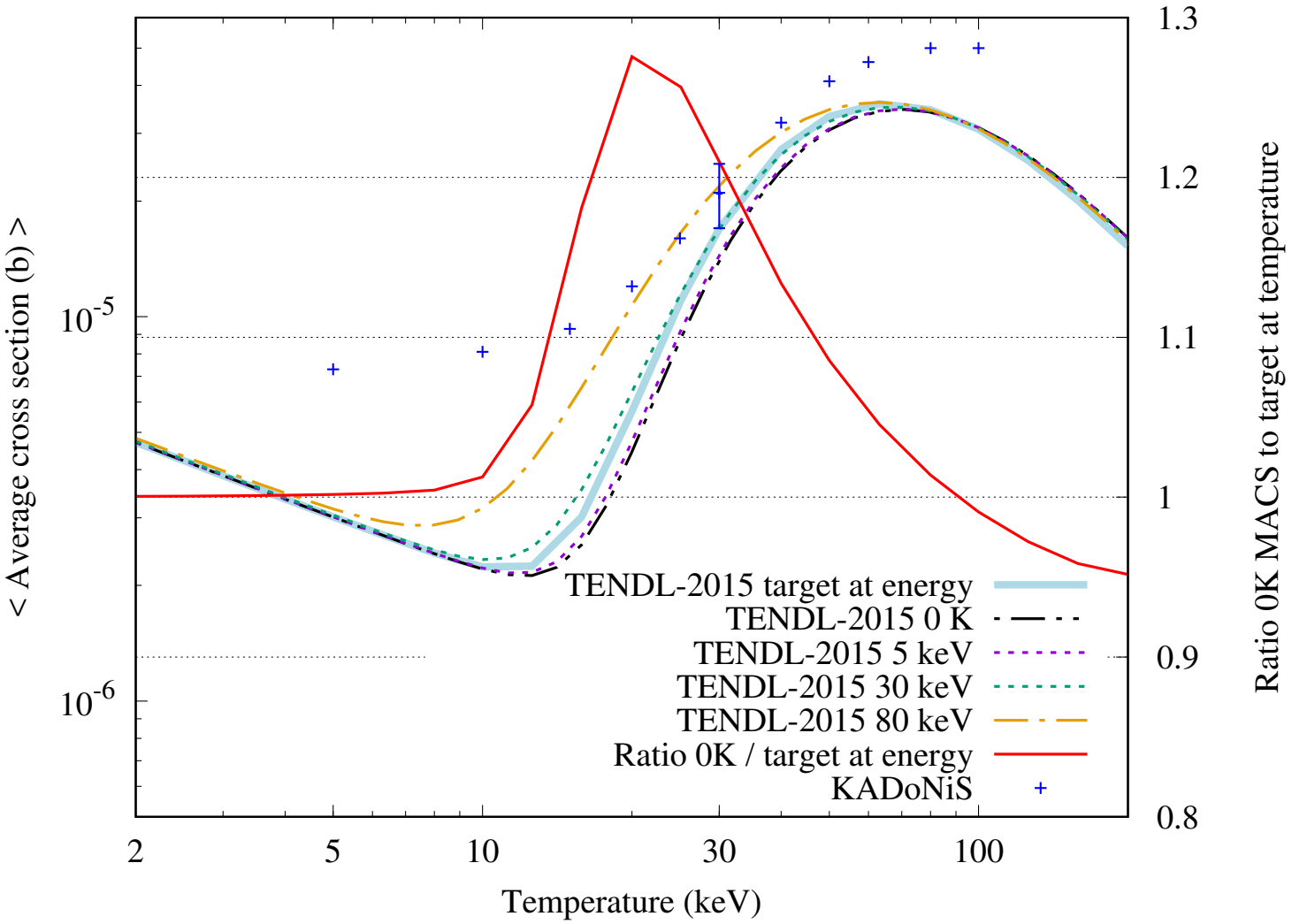
Temperature dependence - C13

Maxwellian-averaged data



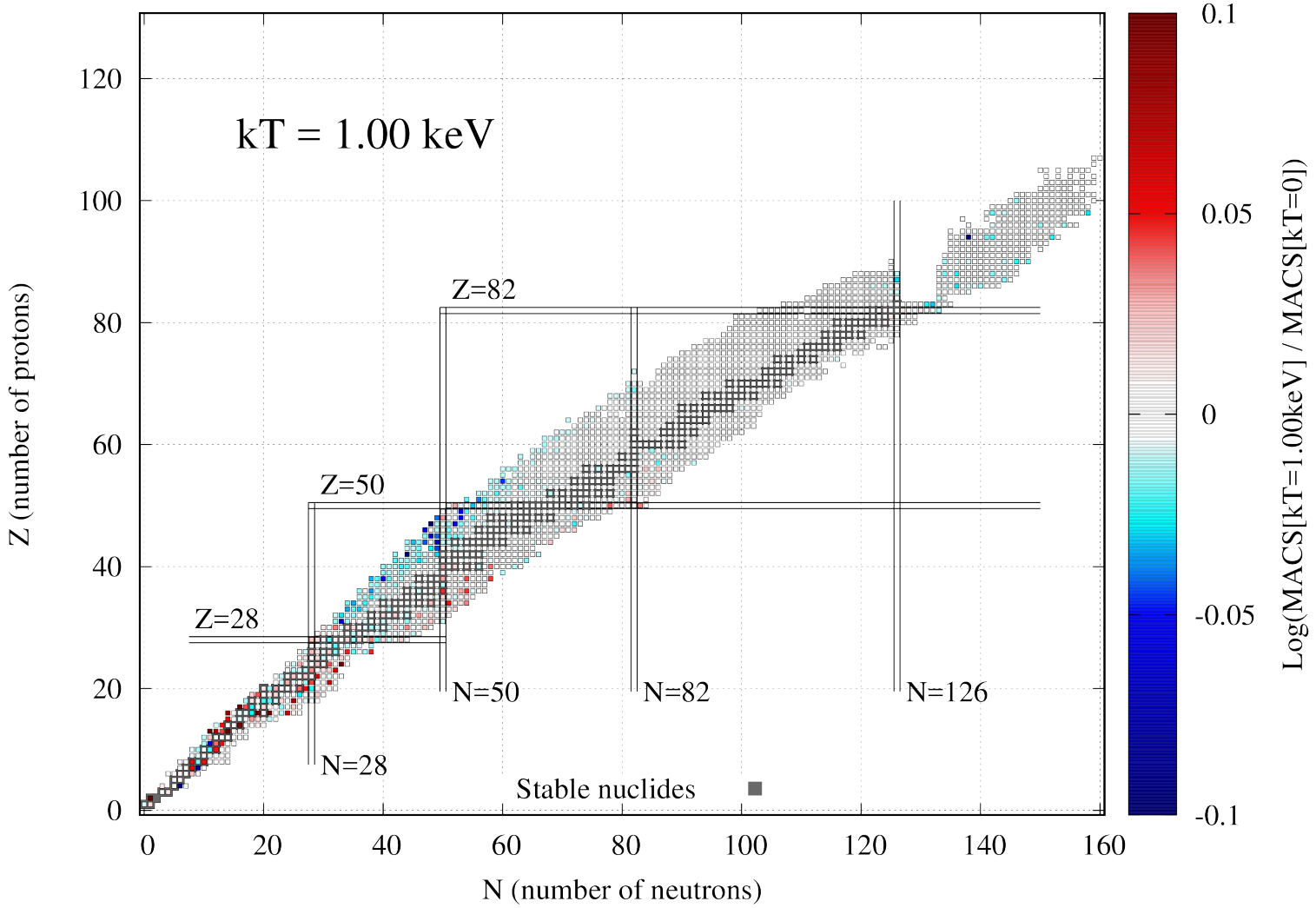
C13 integral values

Maxwellian-averaged data



Temperature dependence - global

Maxwellian-averaged data



FISPACT-II
Upcoming developments

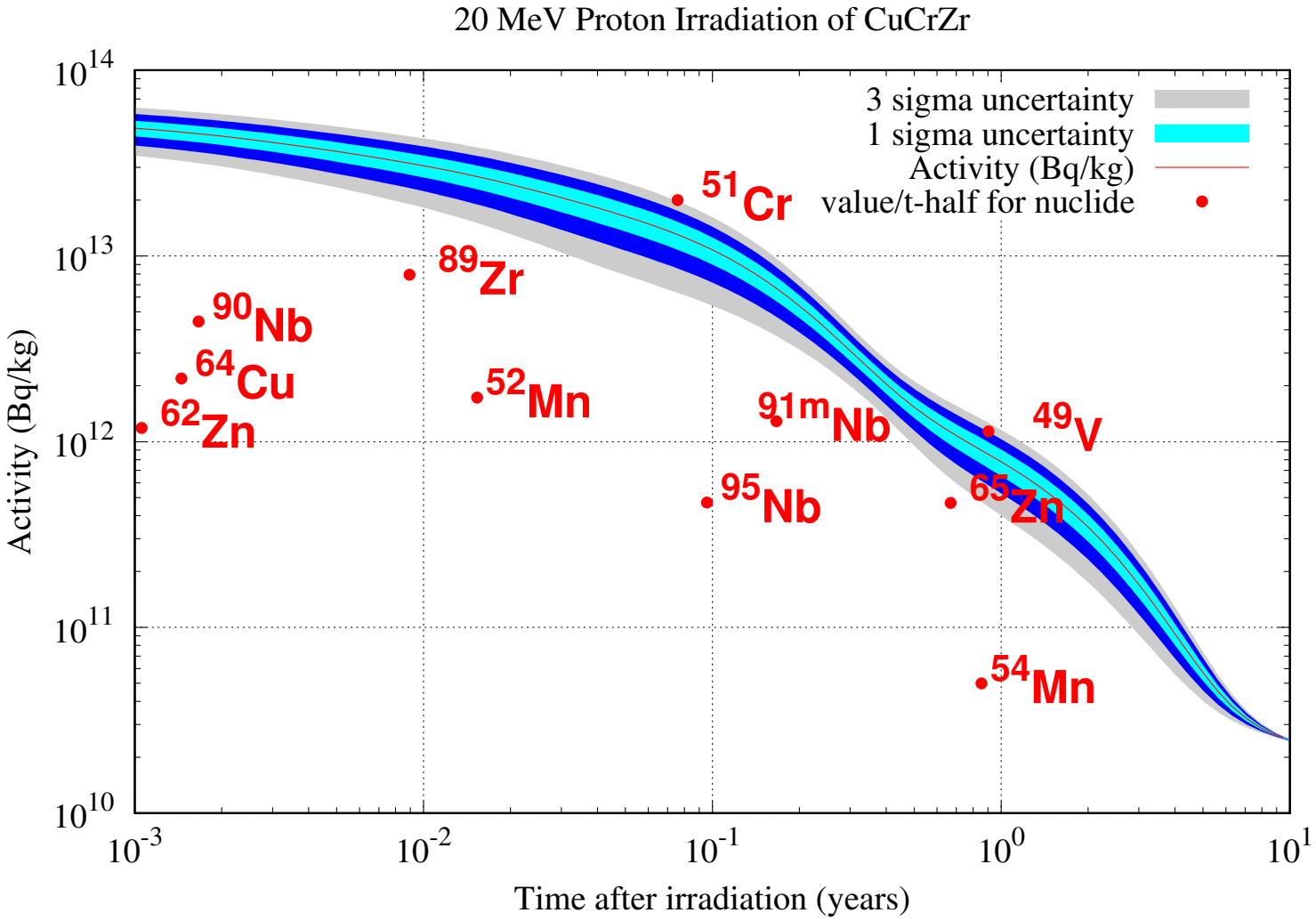
- From 2017, a new programme of development on FISPACT-II has been running at UKAEA, primary topics:
  - Robust code testing system using **continuous integration**, automatically running all tests with line-by-line verification
  - New JSON outputs for automatic post-processing
  - Integration of non-neutron covariances from TENDL-2017
  - Docker containerisation for testing and distribution options
  - High-energy extension data for 200 MeV - GeVs

Non-neutron covariances (I)
Upcoming developments

- Arjan and Dimitri have generated full MF=33 covariances for proton- and gamma-induced reaction data
- Thanks to Jean-Christophe for processing these for FISPACT-II
- These fit within FISPACT-II uncertainty framework, generating pathways and taking all collapsed uncertainties

Non-neutron covariances (II)

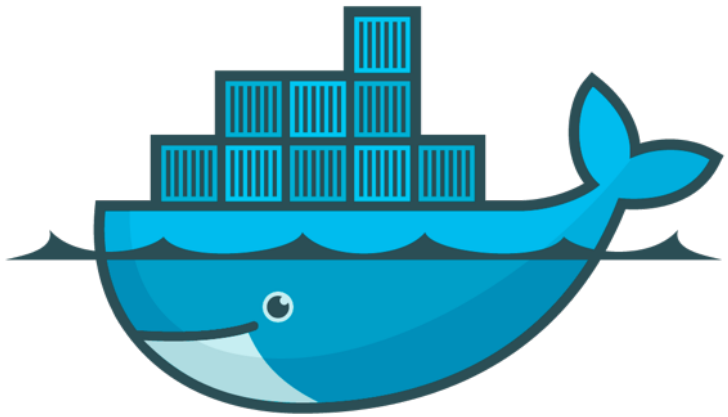
Upcoming developments



Test suite from CI (I)

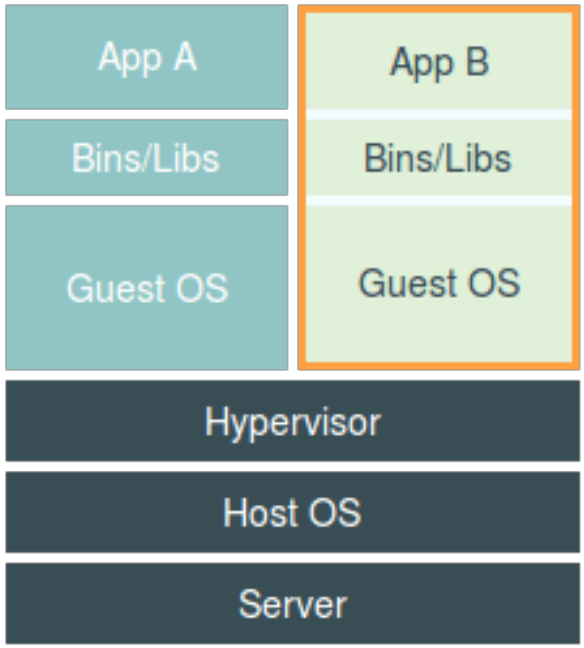
Upcoming developments

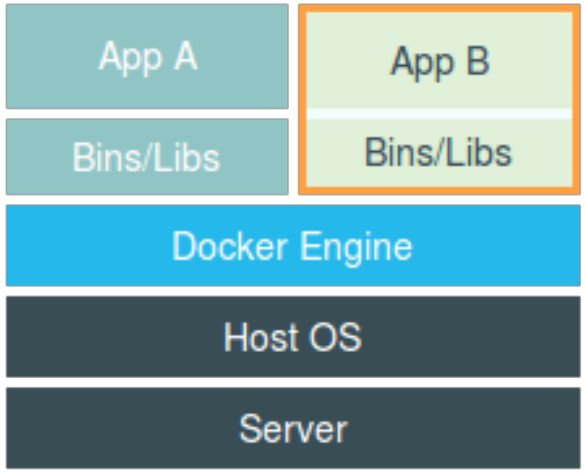
git



docker

Docker containerisation
Upcoming developments

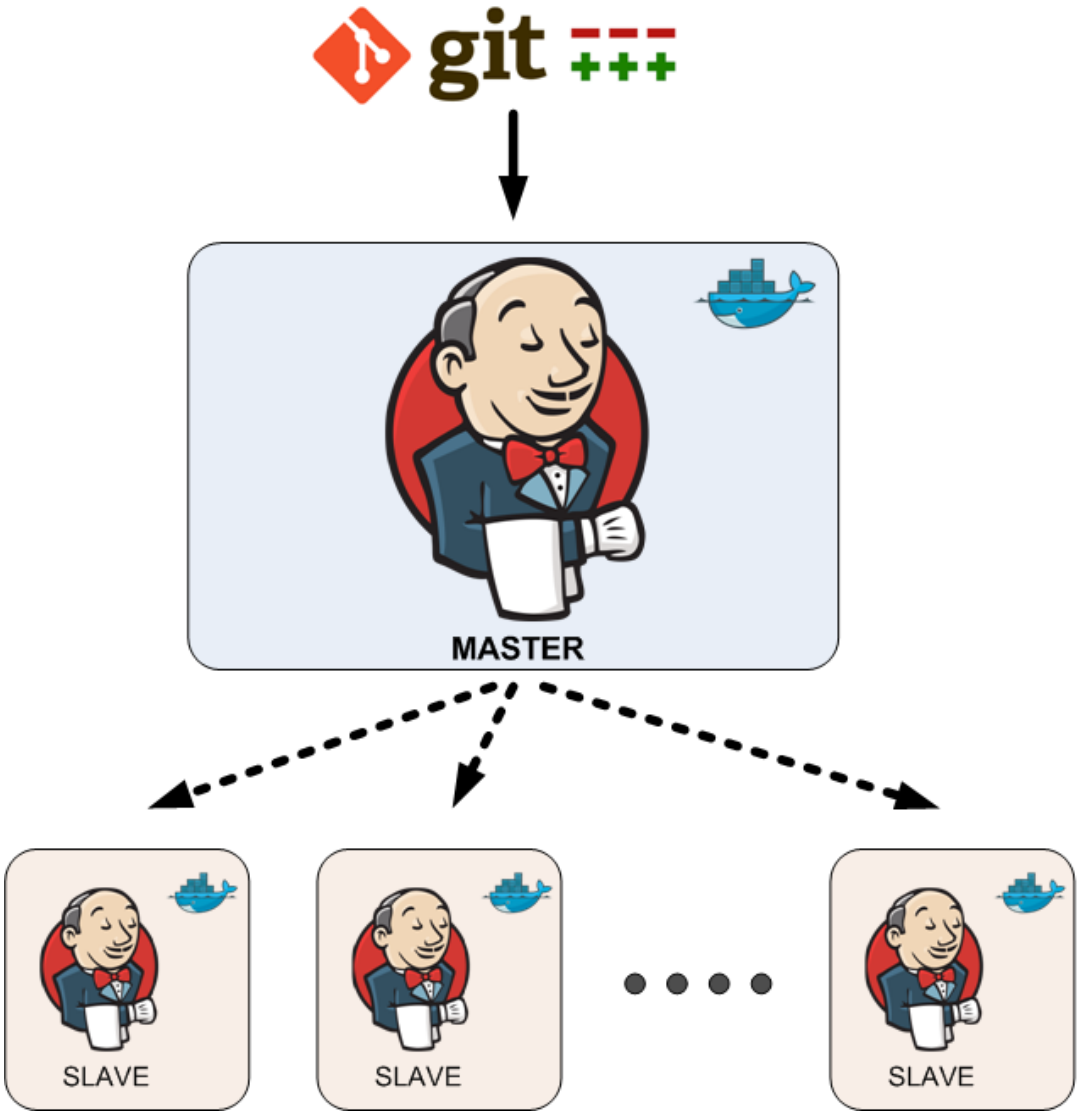




- Offers ability to distribute stable system with libraries, environments, etc.
- `https://hub.docker.com/u/fispact/` (only environments, no code)
- Open source and available for Windows, OS X, Linux

Test suite from CI (II)

Upcoming developments



Requirements & applications

'High'-energy data

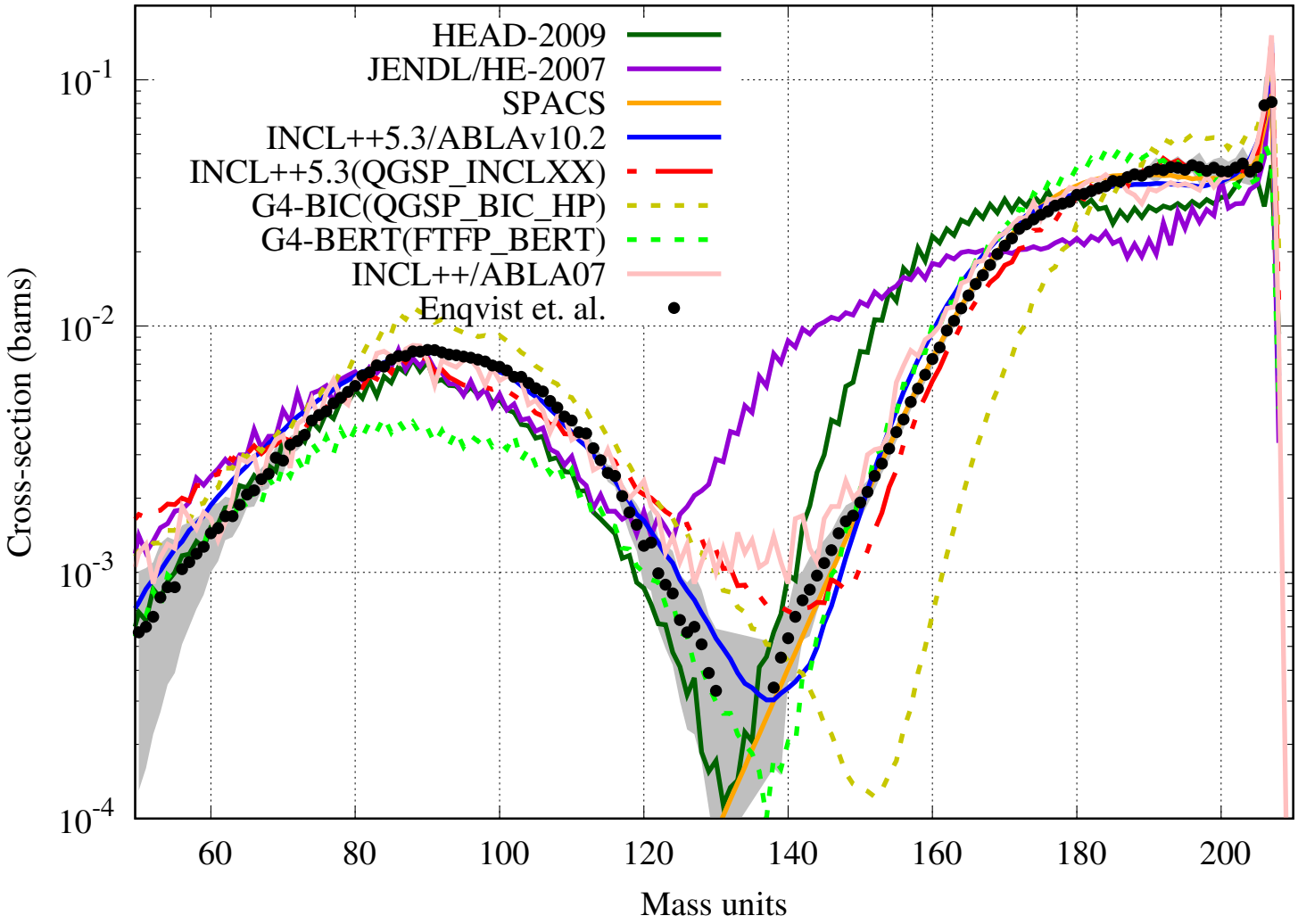
- For activation-transmutation within accelerator-based facilities with incident energies above a few hundred MeV, considerable residual nuclide data is required
- There exist at least two relevant libraries:

Library	Targets	Energy range (MeV)
HEAD-2009	H1-Bi210 (629 files)	150-1000
JENDL-2007/HE	H1-Am242m (106 files)	up to 3000

- Typically, users employ INC+ models within MC codes and these libraries are based on INC+ calculations

Survey of libraries and models - Pb208

'High'-energy data

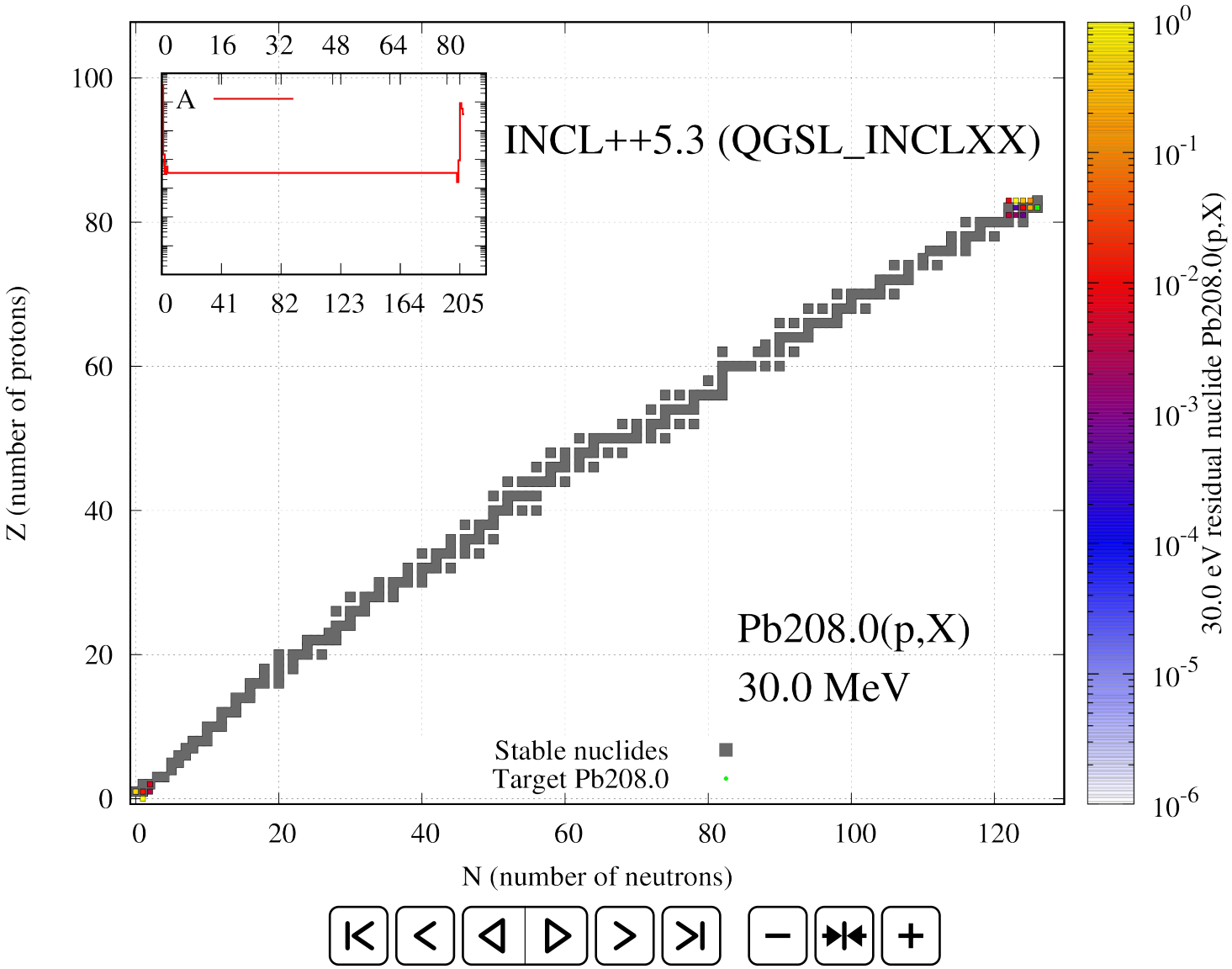


Options moving forward
'High'-energy data

- Many models have poor predictions for mass distributions, which are themselves simple, integral quantities
- We also require full isotopic production and isomers for time-dependent studies
- Full energy range with reasonable discretisation - for example UKAEA 162 group
- The models all require improvement, so the libraries **cannot be set in stone**:
  - Reproducibility: must be able to reproduce without hand modification
  - Traceability: must be able to identify all constituent models/codes/data
  - Completeness: must have all required data – a 'poor' prediction is better than zero

INCL++/ABLA/G4 results

‘High’-energy data



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FISPACT-II - 1GeV W irradiation

'High'-energy data

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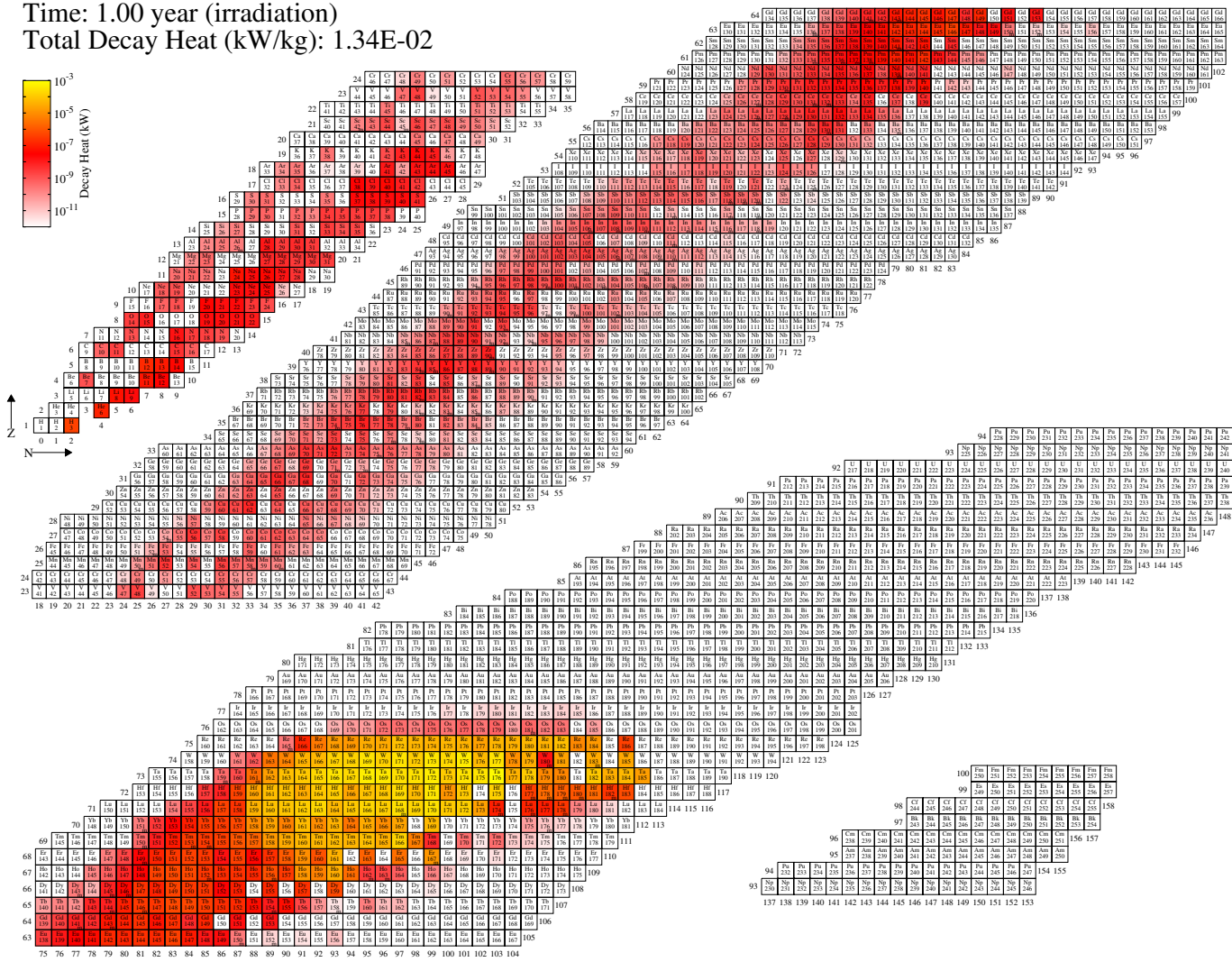

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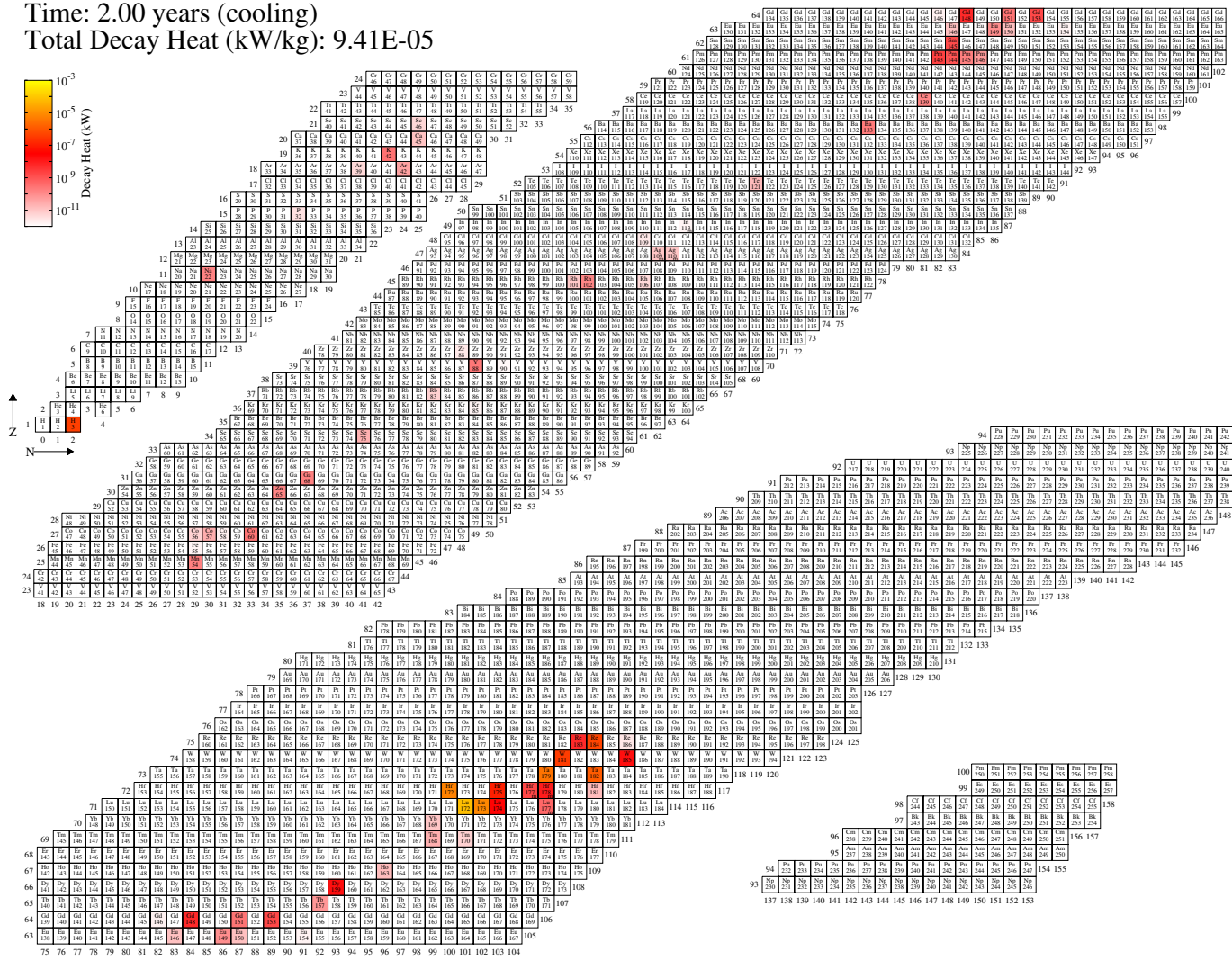

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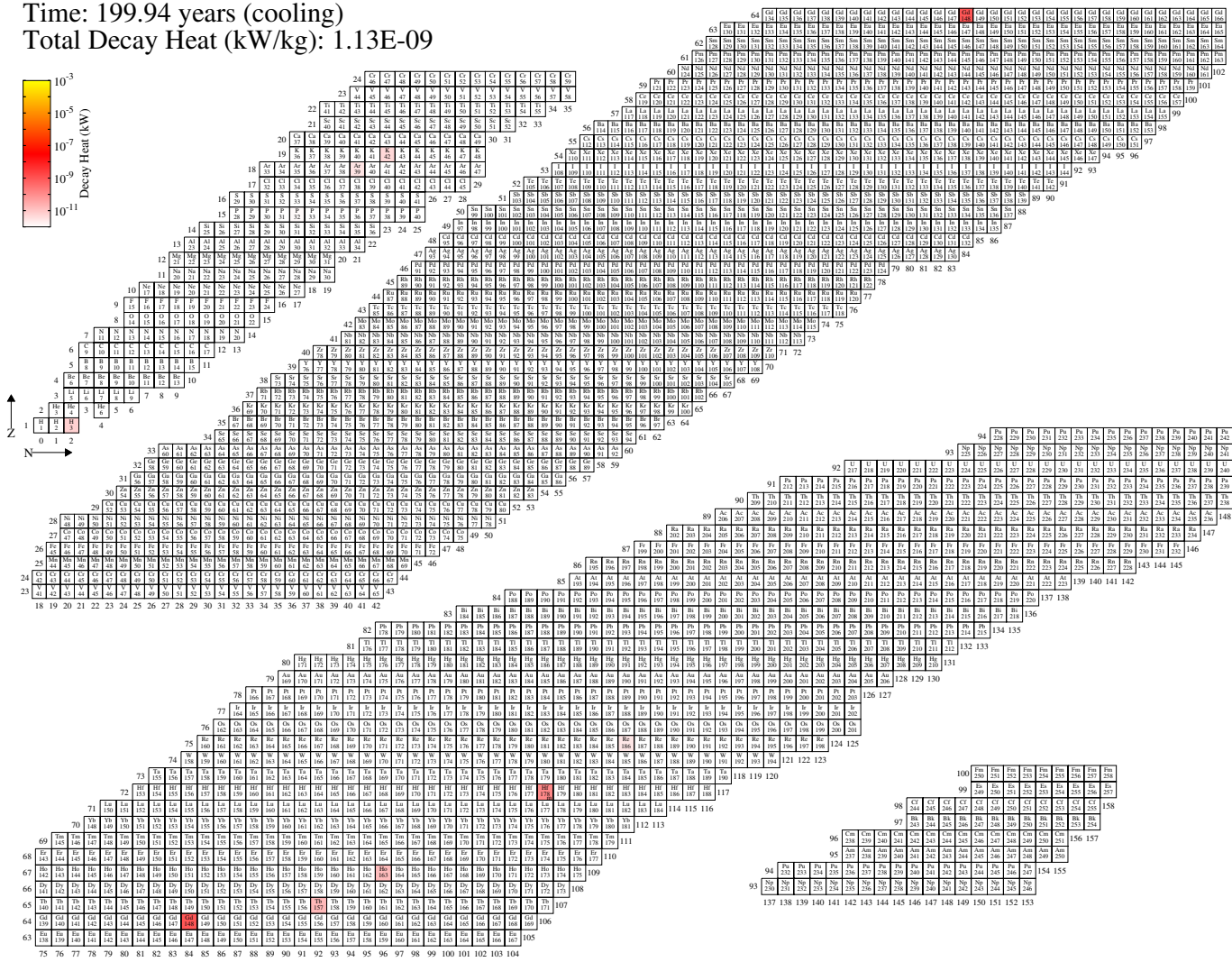

Discussion (I)
'High'-energy data

- Convergence of Monte-Carlo INC model simulations is challenging
  - 256 targets, 36 energies (30 MeV - 1GeV) at 1.0E+6 events = 1000 core-days
- Better option to use TALYS for post-INC:
  - 100 remnants at 1 GeV with spectrum MeV - 100s MeV
  - Pass to TALYS $\rightarrow$ de-excite and fission probability for 100+ fissioning nuclides with energy spectrum MeV - 100s MeV
  - Fission fragments from GEF for each passed back to TALYS to follow to the end (`fy_model=3`)

Discussion (II)

'High'-energy data

- INCL++/TALYS/GEF(/TALYS) calculation offers full data, isotope/isomer production information
- However, per target and incident energy (example 1GeV Pb208):
  - 100+ remnants
  - 100+ remnant excitation energies
  - 100+ non-fission products per remnant per energy
  - 100+ fissioning nuclides per remnant per energy
  - 10+ fissioning energies per fissioning nuclide
  - 1000+ fragments per fissioning nuclide per fissioning energy
- And we want 1000+ targets over 100+ energies
- Age of universe approx 5E+12 days

Conclusions

- FISPACT-II 3-20 currently distributed with TENDL-2015 through OECD-NEA and ORNL RSICC
- FISPACT-II 4-00 will be released in early 2018 with:
  - Latest TENDL-2017 data, including proton/gamma covariances and uncertainty propagation
  - High-energy data forms and simulation capabilities
  - TENDL-2017 V&V reports covering all UKAEA databases
  - Other new libraries (ENDF/B, JEFF, GEF)
  - Many more features, corrections and enhancements

Thank you for your attention

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