NEA
NUCLEAR ENERGY AGENCY

The OECD/NEA Data Bank Computer Program Services (CPS)

Activities on nuclear databases and computer programs

Alice DUFRESNE

Head of the Computer Program Service (CPS), NEA Data Bank

The NEA mission

To assist its member countries in maintaining and further developing, through **international co-operation, the scientific, technological and legal bases** required for a safe, environmentally sound and economical use of nuclear energy for peaceful purposes.

To provide authoritative assessments and to forge **common understandings** on key issues as **input to government decisions on nuclear energy policy** and to broader OECD policy analyses in areas such as energy and the sustainable development of low-carbon economies.

Seeking excellence in nuclear safety, technology and policy

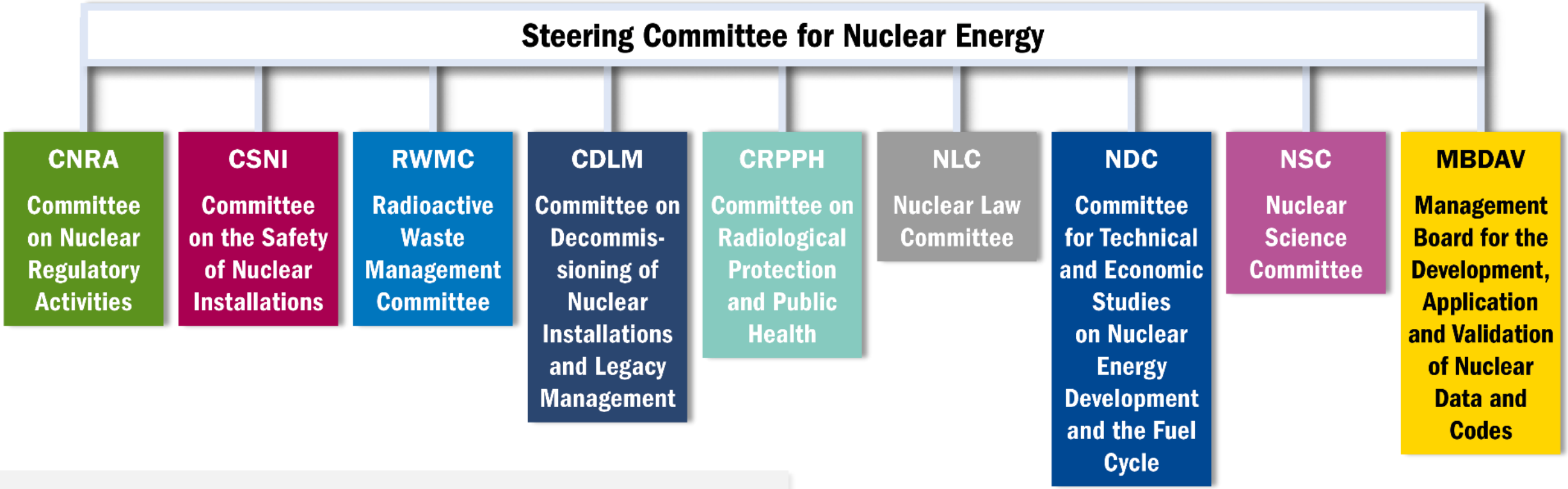
34 member countries + partners
(e.g. China, India, Brazil, etc.)

8 standing technical committees
1 management board
74 working parties and expert groups

26 international joint projects

The NEA Data Bank – a major international resource

NEA committees (as of 1 January 2022)



8 standing technical committees

1 management board

74 working parties and expert groups

Data Bank work areas

The Data Bank is a 'Centre of Reference' for computer codes, nuclear data and knowledge preservation – with MBDAV overseeing the delivery of outputs.

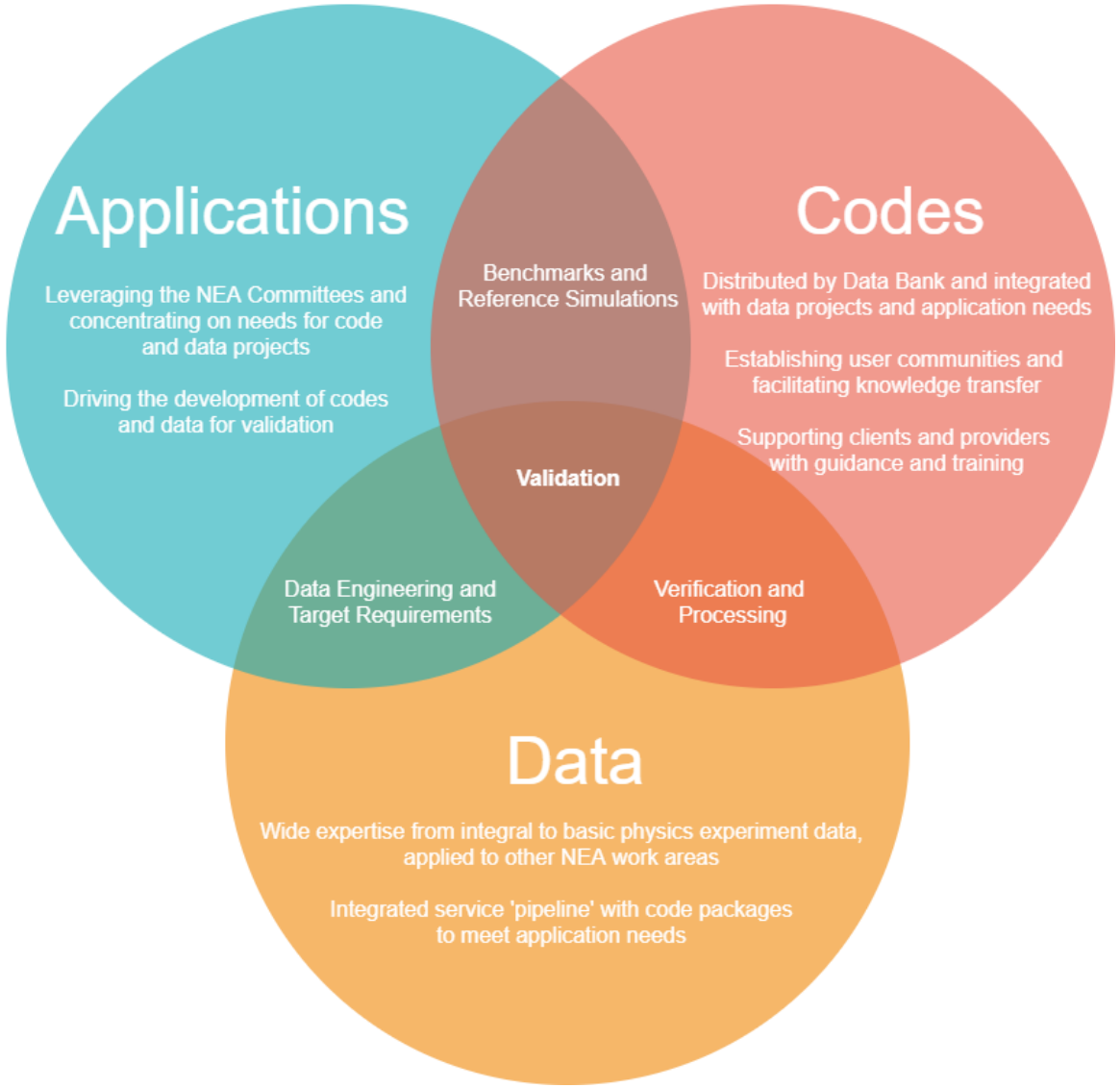
The Data Bank provides **services** benefiting its member countries:

1. **Computer Program Services (CPS):** Acquisition, licensing, testing and distribution of computer codes, and organisation of training courses.
2. **Nuclear Data Services (NDS):** Compilation of measured nuclear reaction data (EXFOR), co-ordination of the Joint Evaluated Fission and Fusion (JEFF) project and related tool development.
3. **Databases of Experiments and Nuclear Knowledge Management:** Preservation and distribution of data (including NEA joint projects and benchmarks) and support for training and educational activities.

Data Bank work areas

Difference between NEA Data Bank and other single-service providers: **all in one place = cross-service potential**

- Basic physics data verified and integrated in codes
- Benchmark models and references for software
- Application target accuracies from stakeholders for modelling and data prioritisation
- Integrated tools and services to support advanced validation

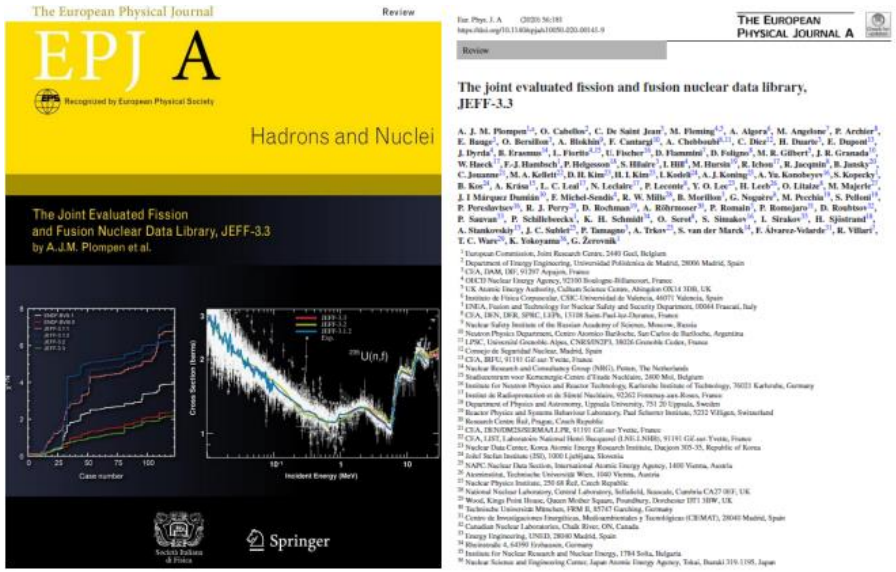


Data Bank Nuclear Data Service (NDS)

- Responsible for compilation of nuclear reaction experimental data for the international EXFOR database (since 1966).
  - Continuing to deliver record numbers of new entries (600+ in 2021).

- Co-ordination and technical support to the Joint Evaluated Fission and Fusion (JEFF) nuclear data library (since 1981).
  - Latest release SOTA "JEFF-3.3" with 80 authors in 36 organisations.
  - New JEFF mandate have already created the first complete 'test' file for JEFF-4.0, using modern evaluation methods.

- Developing tools for the compilation, visualisation and testing of nuclear data, including resources used by clients for nuclear data and code validation.
  - Java-based Nuclear Information System (JANIS).
  - Since 2021, Data Bank staff have begun using an NEA-hosted GitLab platform to integrate data development and testing, with a plan to leverage the suite of NEA SCI-developed benchmark databases and applications.

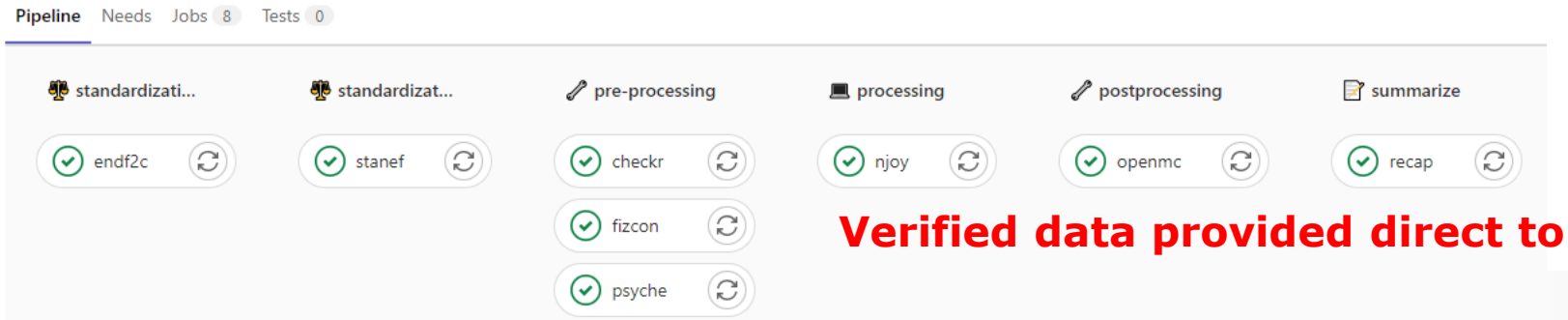


NDS: JEFF reform

- 12 newly established technical groups and a project review group for the Co-ordination Group
- Technical session Chairs brought energy and insight, working closely with NEA Secretariat to create technical agendas
- New approach including technical focus groups with topical sessions:

1.	Random files for uncertainty	23 Feb 2022
2.	Special purpose libraries (e.g. activation)	8 Mar 2022
3.	'Big 3' and JEFF-4 roadmap	22 Mar 2022
4.	Processing pipeline	31 May 2022
5.	Fission yields and covariances	16 Jun 2022
6.	Validation framework	22 Jun 2022
7.	Comparison of REFIT-SAMMY-CONRAD	TBD
8.	General-purpose Covariances	19 Sep 2022
9.	Dedicated iron evaluation and testing	TBD
10.	Pipeline HACKATHON	14-15 Sep 2022

- And adoption of GitLab-based workflows to manage the project, test the data in real time and directly integrate it with computer codes within the CPS catalogue (see next slides)



Verified data provided direct to software partners

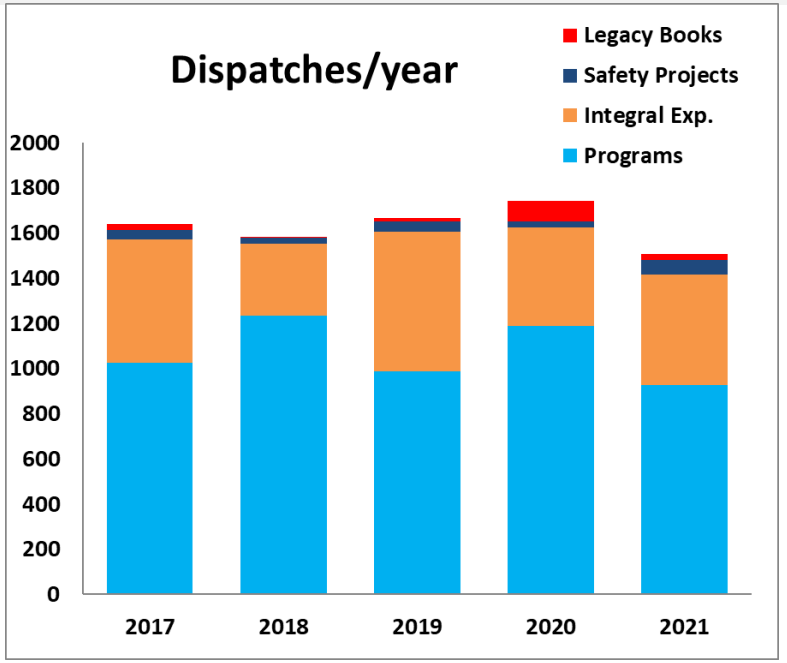
Data Bank Computer Program Service (CPS)

- Originally dedicated to codes, but now also covering the preservation and distribution of most NEA restricted content, incl. safety joint-projects and **benchmark outcomes, integral experiments, handbooks**, etc.

- International network of users (28 NEA Data Bank countries + arrangements with RSICC and IAEA)
  - ➢ 900+ nominated establishments in the 28 NEA Data Bank participating countries.

- CPS acts as a visible distribution centre, following the conditions set by the owners. CPS distributes 1600+ packages/year (of them, ~1000 are codes).

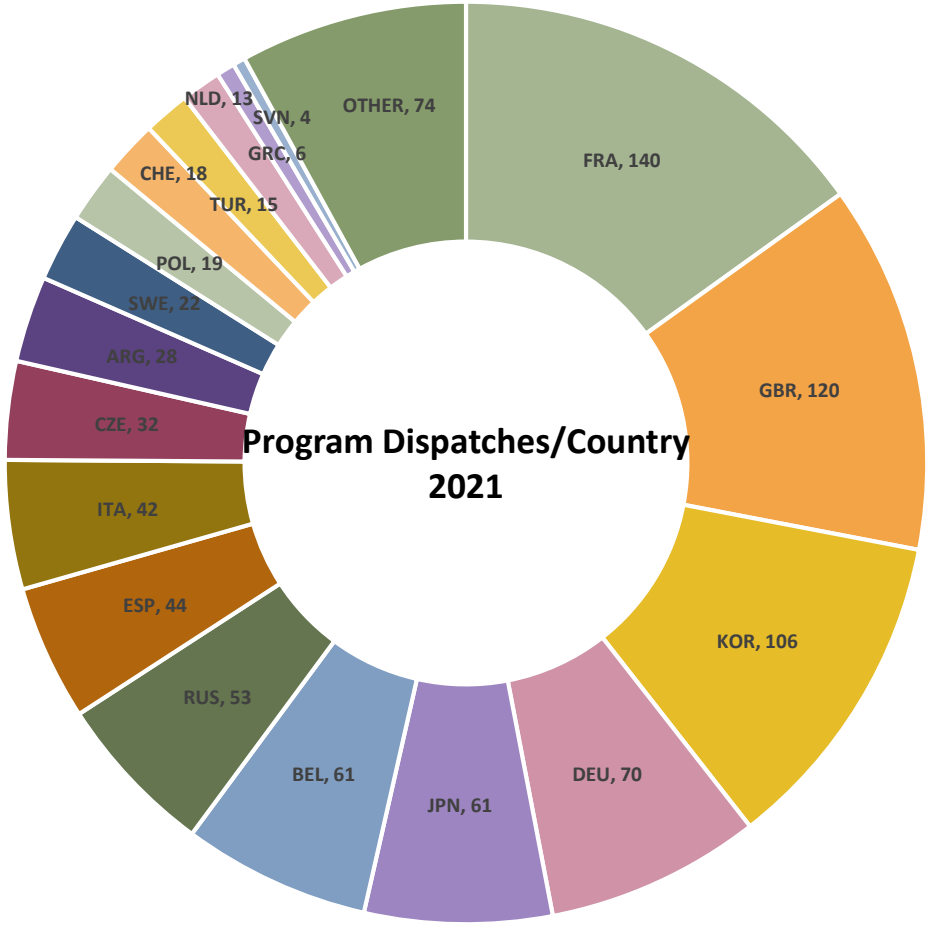
- CPS organises training courses on the widely used codes, at the NEA and other institutes. Typically ~10+ courses/year, gathering ~150 participants in total.



Year	Programs	Integral Exp.	Safety Proj.	Legacy Books	Total
2017	1024 (62%)	547 (33%)	41 (3%)	28 (2%)	1640
2018	1234 (78%)	317 (20%)	27 (2%)	5 (0%)	1583
2019	986 (59%)	618 (37%)	47 (3%)	15 (1%)	1666
2020	1188 (68%)	438 (25%)	26 (1%)	90 (5%)	1742
2021	928 (62%)	488 (32%)	66 (4%)	24 (2%)	1506

CPS network

- Number of LO: 924 last end May
- Every year, every DB country receives computer programs from CPS



Country	Nb of LO
Japan	274
France	91
Germany	76
Spain	68
United Kingdom	57
Italy	50
Russia	46
Korea	41
Sweden	34
Belgium	22

CPS most distributed programs – 2021

Global numbers

	Nb of distrib.	Program Name	Country of Origin
1	144	SCALE 6.2.4	United States
2	110	FISPACT-II 5.0	United Kingdom
3	73	SERPENT 1.1.7	Finland
4	55	VISUAL EDITOR 61	United States
5	42	PENELOPE2018	Spain
6	32	SUPERMC 3.3.0	China
7	22	ADVANTG 3.2.1	United States
8	21	FISPACT-II 4.0	United Kingdom
9	20	COBRA-SFS 6.0	United States
10	17	ADVANTG 3.0.3	United States
11	14	PENGUIN	Spain
12	11	CRISTAL V2.0.3	France
13	10	ORIGEN-ARP 2.00	United States
14	10	QAD-CGGP-A	United States

Numbers for Spain (2021-2022)

Nb of distrib	Program Name	Country of origin
21	SCALE 6.*	United States
13	PENELOPE2018	Spain
4	FISPACT-II *	United Kingdom
4	PENGUIN	Spain
4	SERPENT V2.2.0 -R-	Finland
4	SUPERMC 3.3.0	China
3	COBRA-SFS 6.0	United States
3	FINPSA TRAINING2.1-R	Finland
3	SCEPTRE 1.7	United States
3	VISUAL EDITOR 61	United States
2	ARCON96	United States
2	UMG 3.3	Germany
2	ZZ-NMF-90	IAEA

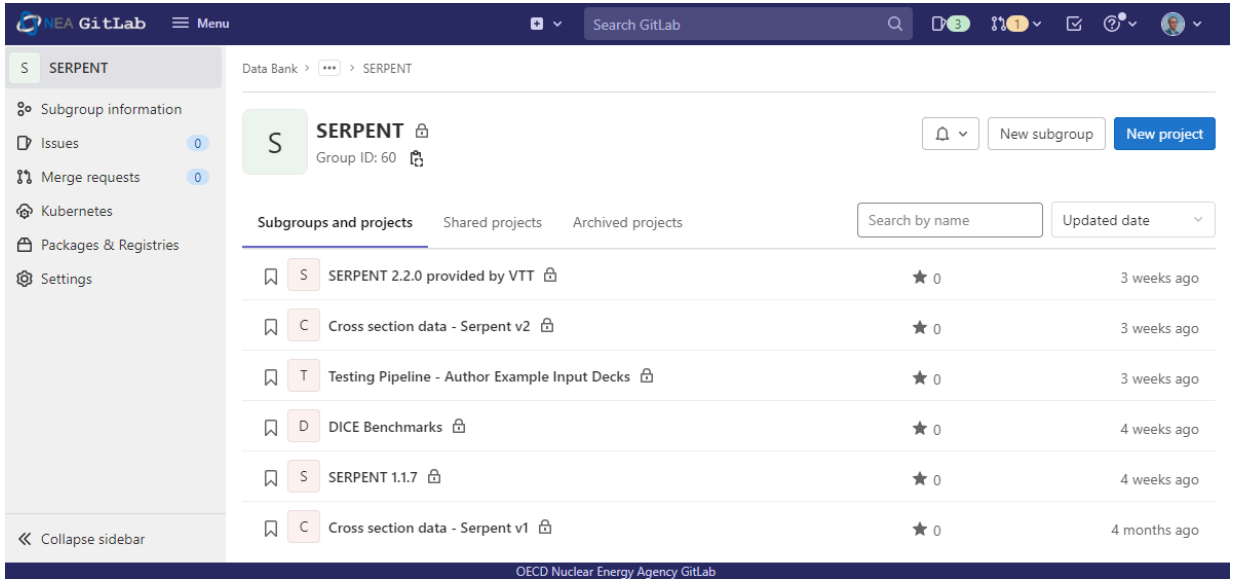
Contributions from Spain to the CPS collection

Program Name	Last updated	Contributor
ZZ-AMPXJEFF3.1.1UPM	16-Sep-22	Universidad Politecnica de Madrid
ZZ-AMPXJEFF3.3-UPM	16-Sep-22	Universidad Politecnica de Madrid
PENGUIN	11-Mar-20	Universitat de Barcelona
PENELOPE2018	24-Jan-20	Universitat de Barcelona
ZZ-TSL-ACE/2013	5-Mar-14	Universidad Politecnica de Madrid
MCUNED	11-Jul-13	Universidad Nacional de Educacion a Distancia
ACAB-2008	5-May-11	UNED & UPM

Nb of distrib (2021-2022)	Programme name
87	PENELOPE2018
30	PENGUIN
2	ACAB-2008
2	MCUNED
2	ZZ-TSL-ACE/2013

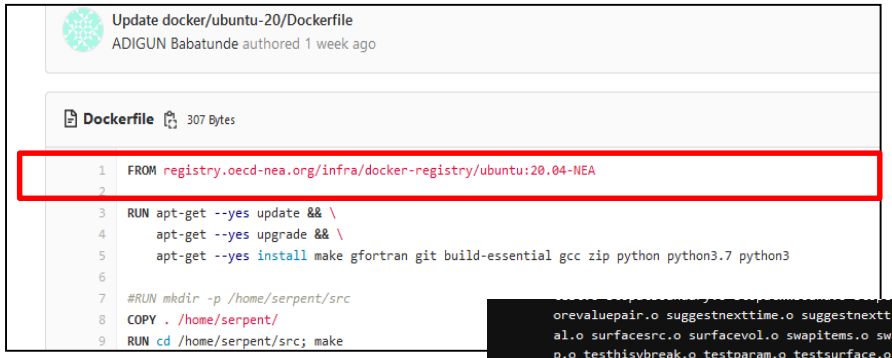
CPS new working methods

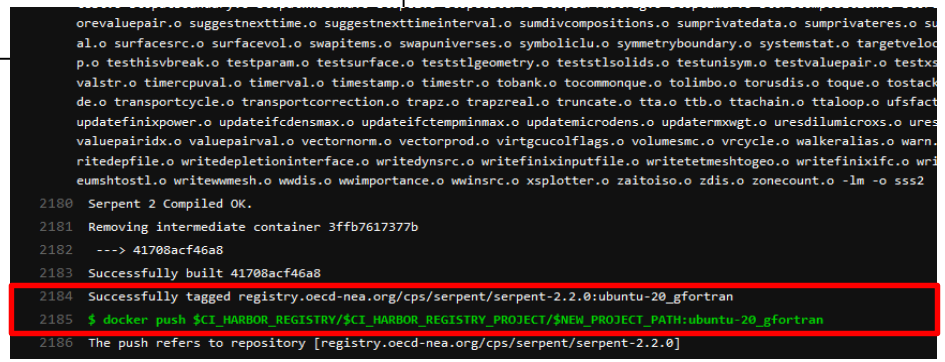
- Direct engagement with developers through the NEA GitLab NOT to ‘only’ use the GitLab platform as a repository service, but to leverage several other services:
  - Move CPS testing into a transparent, collaborative and reproducible system
  - Containerise code for use in other NEA pipelines (e.g. data processing, benchmarks)
  - Create portable images with code (and/or other content) for a range of user needs, including education and training activities
- Example – release in May 2022 of Serpent-2 (VTT, Finland) Monte-Carlo code

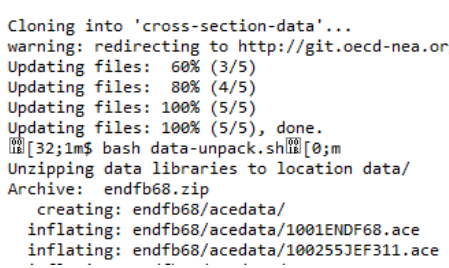


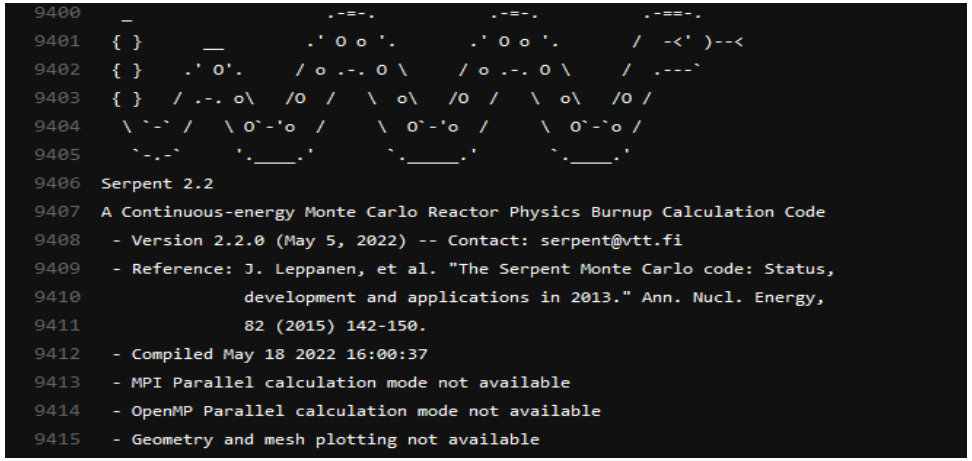
CPS new working methods (II)

- Reproducible container configuration, automatically processed @NEA GitLab
- Images built, stored, and available for internal pipelines or distribution w/Harbor
- Nuclear data directly integrated at image level for testing, distribution and end-use
- Complete testing environment for developers of code/data with real-time feedback









Added value of the CPS distribution

1. Visibility

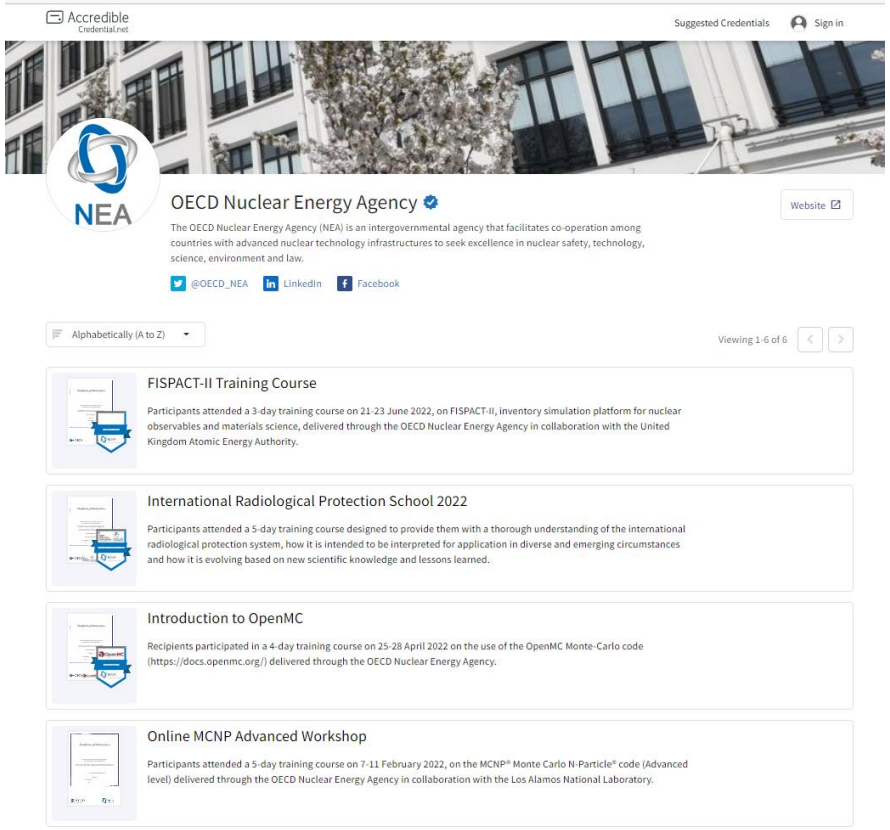
- open or restricted distribution, with a framework flexible enough to accommodate country-specific export control restrictions
- to an international network of users (2500+ users among the NEA Data Bank countries)

2. Integration in the Data Bank ecosystem, that include codes, data and applications

- Benchmark models and references for software
- Application target accuracies from stakeholders for modelling and data prioritisation
- Integrated tools and services to support advanced validation

3. Integration in the training programme and the "eLearning" initiative

- NEA has installed a Learning Management System, coupled with a credential issuing platform – towards having an NEA catalogue of courses and certificates
- Development of educational resources, in connection with a training or possibly self-paced training



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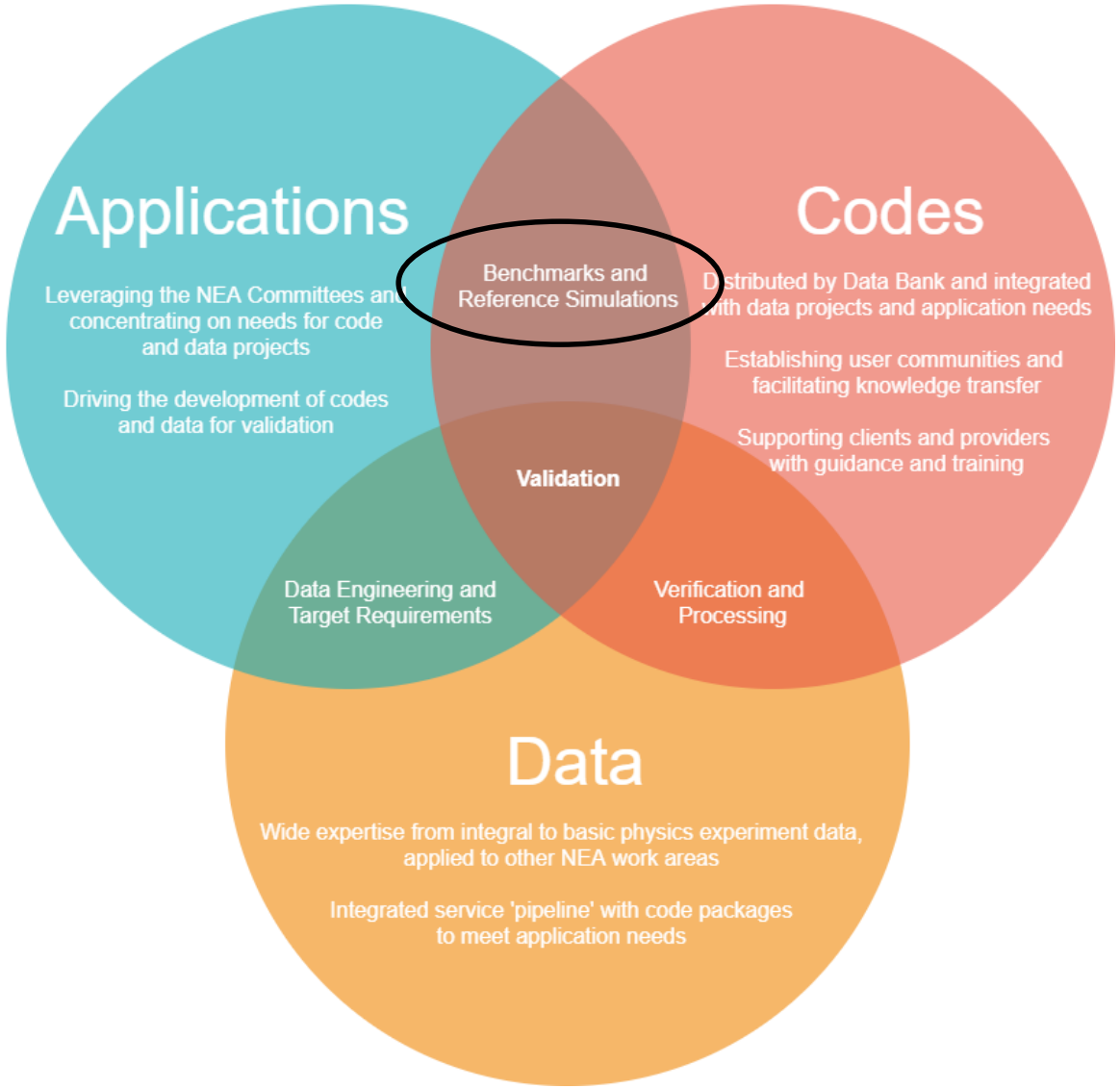
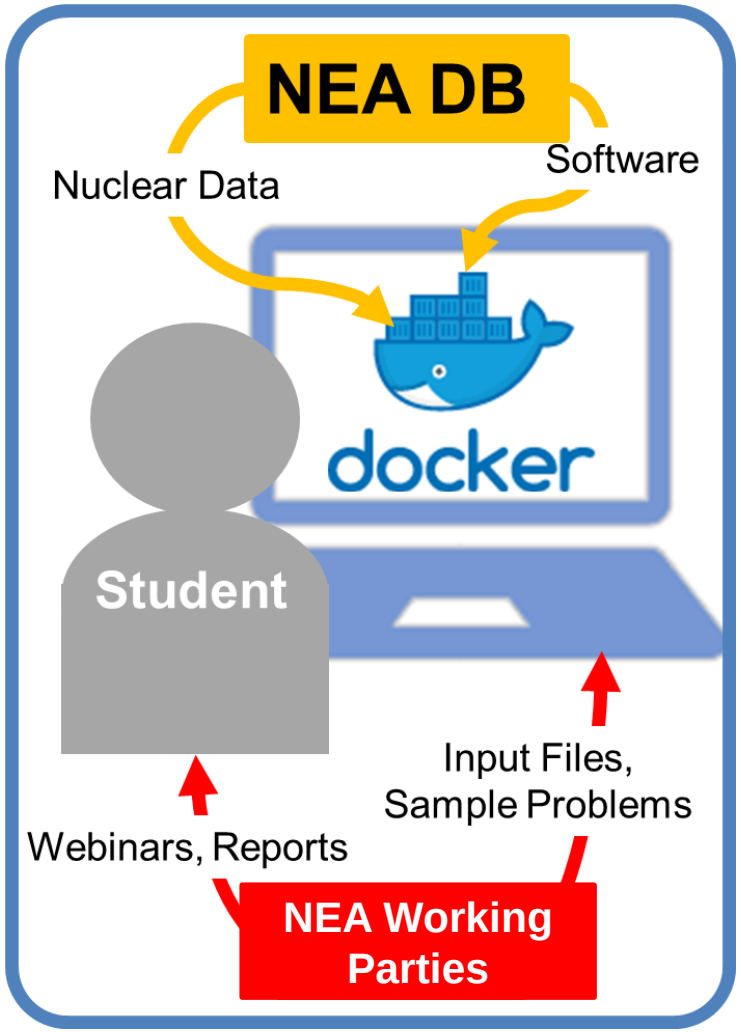
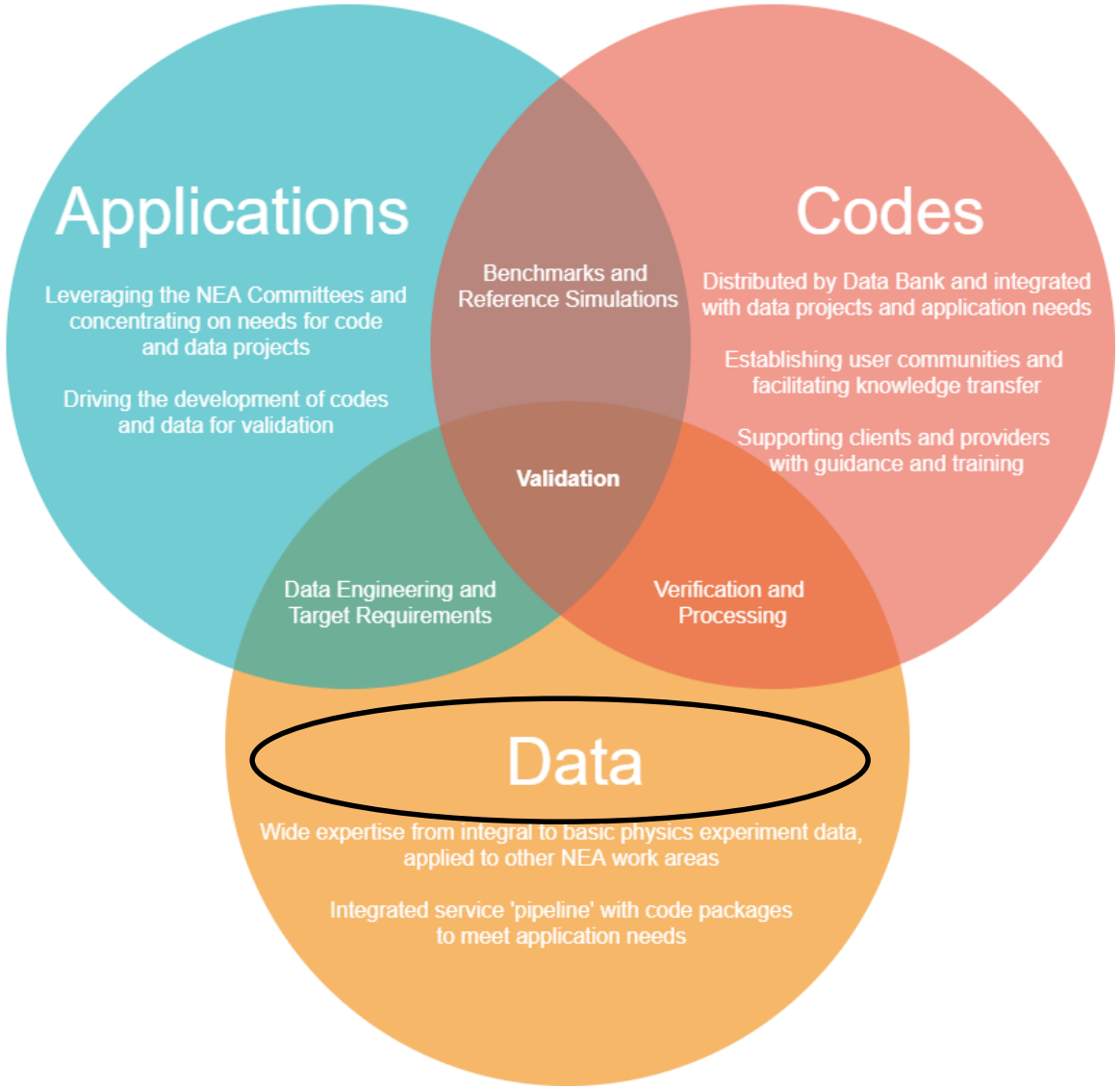


Collaboration on Benchmark Projects

- Leveraging the capabilities of code and data containerised environment, including as a support for education and training activities
- Internal collaboration between SCI and DB on benchmarks to standardise and simplify distribution and access rules, and to classify benchmark activities
- Users will be able to access codes, data, benchmarks and be informed of relevant training activities, through public-facing pages, that will direct them to relevant materials
- Benchmark expert engagement key to content population
- Newly acquired code packages and upcoming releases through DB will help support this initiative
- Area for engagement with STCs and MBDAV members to help expand access for more software packages to improve the catalogue of potential simulation systems





ICSBEP TRG Technical Review Group for the International Criticality Safety Benchmarks Evaluation Project

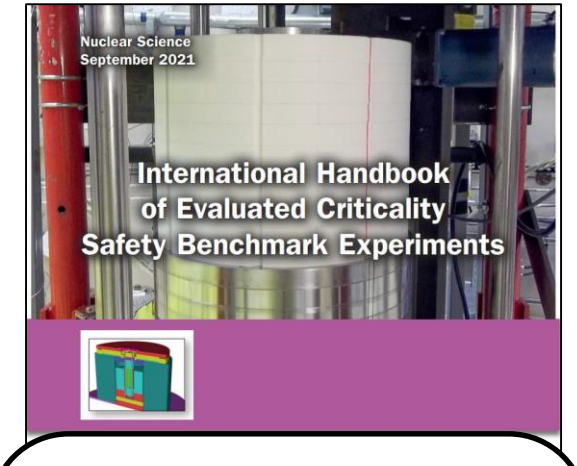
(New) Chair: C. Percher (LLNL, USA) – (New) Vice-chair: W.J. Marshall (ORNL, USA) – Secretariat J.-F. Martin

The ICSBEP continues to provide high-quality integral benchmark data

- Valuable for nuclear data testing, uncertainty reduction, criticality safety, reactor physics, advanced modeling and simulation
- Data and expertise contributed from 26 countries
- Enable current and future activities supported by experimental validation

2021 Edition

- Following TRGs end of 2020
- ~80,000 pages, 587 evaluations, incl. 5 new and 10 rev.
- Available soon
- DICE, Database for ICSBEP maintained and annually released



oe.cd/nea-icsbep
www.oecd-nea.og/dice

2022 Edition

- Annual meeting in Oct.&Dec 2021
- ~80 participants
- 10 new evaluations (7 approved) + 1 rev.
- Editing in progress

Next ICSBEP TRG: April 2023

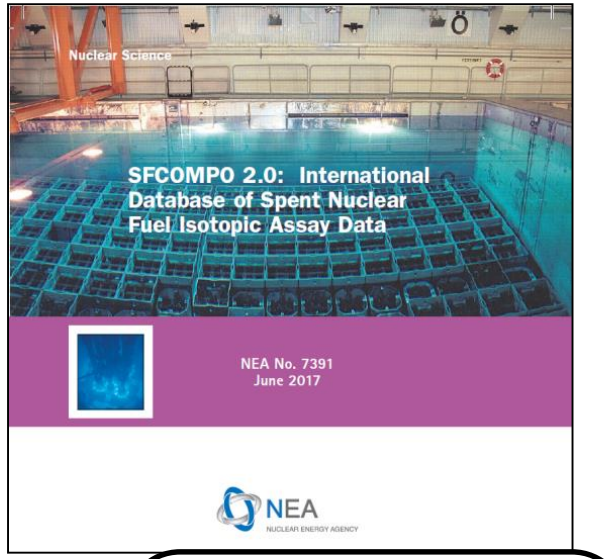
SFCOMPO TRG Technical Review Group for the International Assay Data of Spent Nuclear Fuel Database

Chair: G. Ilas (USA) – Secretariat J.-F. Martin

SFCOMPO 2.0 **is the largest international database of open experimental radiochemical assay data for spent nuclear fuel** - over 700 spent nuclear fuel samples from fuel irradiated in 44 reactors

1. Collection of experimental data incl. decay heat data
   - Continuously adding **publicly available decay heat data**
   - Progress on data release by the MALIBU program participants with support of SFCOMPOTRG, in view of adding to the SFCOMPO2.0
   - Scheduled addition of REGAL data
2. **Evaluation of the experimental data and the development of benchmarks and benchmark models**
   - 3 in progress: Fukushima Daini 2, BWR samples SF98 and SF99; Gösgen PWR GU4, Fukushima Daini 8x8-4
   - 2 approved: TMI1 assemblies NJ05YU and NJ070G (15x15); Fukushima-Daini1 2F1 and 2F1ZN3 (9x9)
   - Incl. benchmark models with quantified uncertainties
3. Maintenance of the database and GUI

>> Maintaining and developing interactions with Nuclear data, Fuel cycle and RadWaste activities



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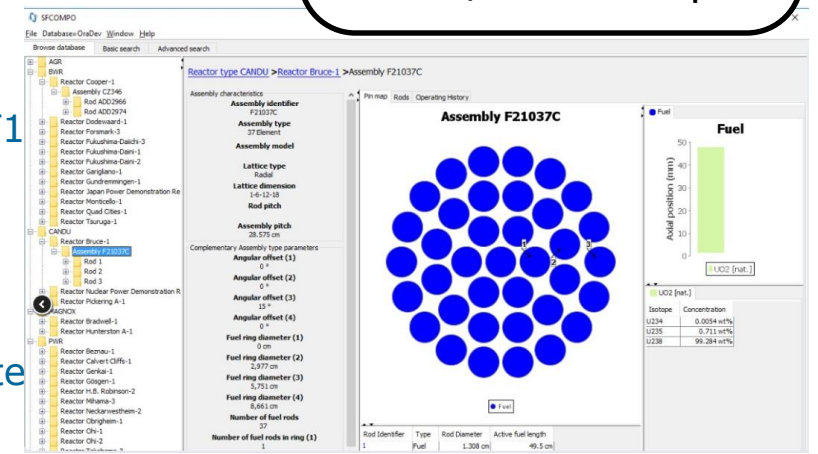
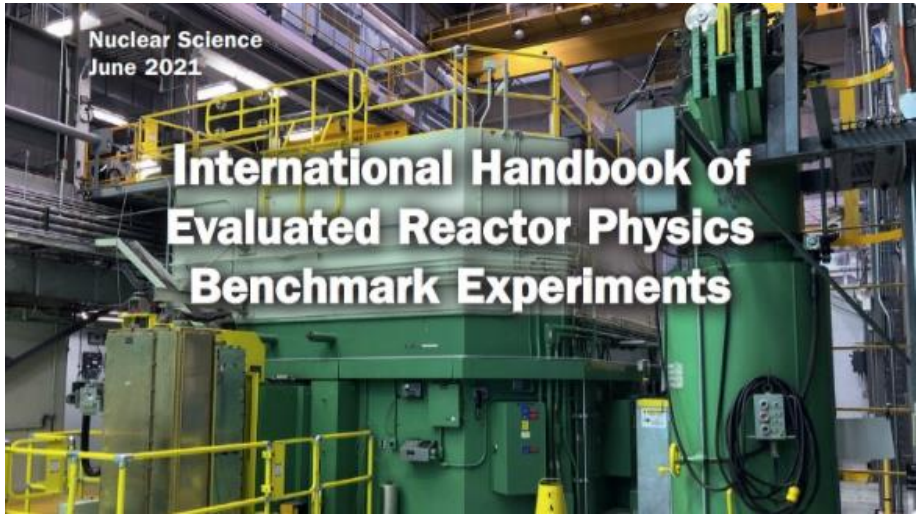


International Handbook of Evaluated Reactor Physics Benchmark Experiments Technical Review Group (TRG)

(New) Chair: M. DeHart (USA) – Secretariat I. Hill

- 2021 TRG Meeting was held in December:
  - IPEN evaluation on kinetics parameters and reactivity effects
  - Revision to ZPPR evaluations to clarify drawer orientation
  - Updates on TVA-WB1 and MPCMIV benchmark evaluations
- Next meeting is scheduled to be held in April 2023 in conjunction with the ICSBEP TRG.



Next Handbook Edition:

- 23 Participating Countries
- 56 Reactor Facilities
- Data from 169 Experimental Series
  - 165 Approved Benchmarks
  - 4 DRAFT Benchmarks
- Available Soon

International Handbook of Evaluated Reactor Physics Benchmark Experiments Technical Review Group (TRG)

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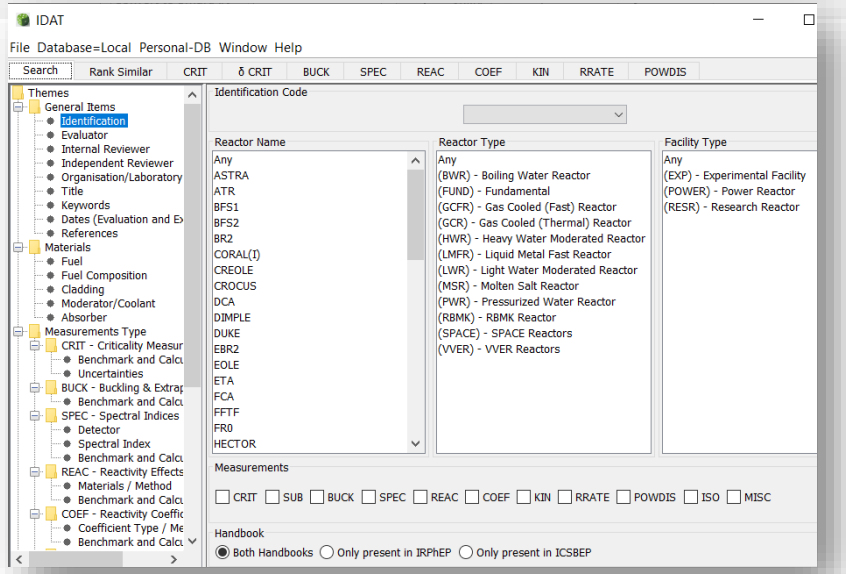
  - Updates on TVA-WB1 and MPCMIV benchmark evaluations
- Next meeting is scheduled to be held in April 2023 in conjunction with the ICSBEP TRG.
- NEA continues to maintain the relational database tool to search the Handbook: www.oecd-nea.org/idat
  - IDAT allows users to search and interrogate the handbook for experimental configurations and data to support applications



Facility	Spectrum	Ratio		Rough Uncertainty
BFS1	Fast	Am^{241f}, Am^{243f}, Cm^{244f}, Cm^{245f}, Np^{237f}, Pu^{239f}, Pu^{240f}, Pu^{241f}, Pu^{242f}, Th^{232f}, U^{238c}, U^{238f}	Pu^{239f}, U^{235}	~3%
BFS2	Fast	Pu^{239f}, U^{235f}, U^{238f}	Pu^{239f}, U^{235}	~3%
DCA	Thermal	U^{238} **factor		~5%
DIMPLE	Thermal	Pu^{239f}, U^{238c}, U^{238f}	U^{235}	~1%
FFTF	Fast	H^1-Elastic, neutron spectrum	-	~Variable wrt Energy
IPEN	Fast	Cadmium ratio, other ratios	-	~1%
LR(0)	Thermal	H^1-Elastic neutron spectrum	-	~1%
PROTEUS	Thermal	Np^{237c}, Th^{232c}, Th^{232f}, $Th^{232N,2N}$, U^{233f}, U^{235f}, U^{238c}, U^{238f}	Pu^{239f}, Th^{232c}	~2%
SCCA	Fast	(Cd ratio)		~2%
SNEAK	Fast	Pu^{239f}, U^{238c}, U^{238f}	U^{235f}	~3%
SSCR	Thermal	Dy^{164c}		~5%
ZEBRA	Fast	H^1-Elastic neutron spectrum Li Time-of-flight Pu^{240f}, Pu^{241f}, U^{235f}, U^{238c}, U^{238f}	Pu^{239f}, U^{235f}	~3%
ZPPR	Fast, Intermediate	H^1-Elastic neutron spectrum, U^{235c}, U^{235f}, U^{238c}, U^{238f}	Pu^{239f}, U^{235f}	~3%
ZPR	Fast, Intermediate	U^{235f}, U^{238c}, U^{238f}	Pu^{239f}, U^{235f}	~3%
ZR6	Thermal	Ce^{143c}, Dy^{164c}, In^{115c}, Mn^{55c}, U^{235f}, U^{238c}	-	~2%

News on SINBAD – on-going Task Force

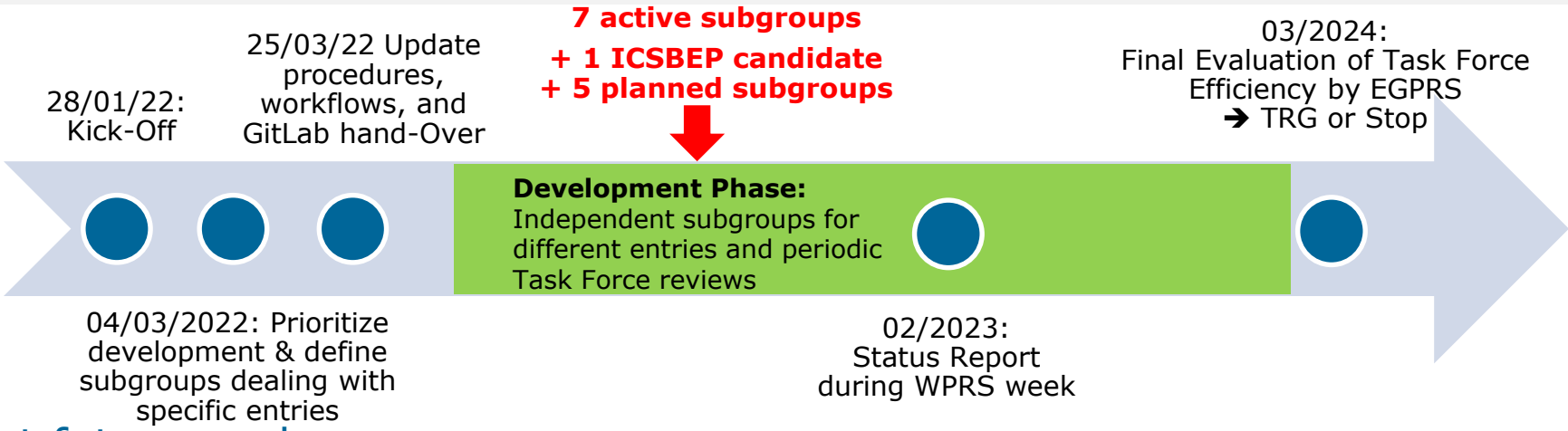
Chair: T. Miller (USA) – Secretariat O. Buss

- Modular organisation: subgroups working on different entries/experiments
- Progressive, well-defined process: SINBAD entries can undergo subsequent updates to reach well-defined intermediate maturity levels with well-defined prerequisites – see the Maturity Level Scheme
- Goal to update publicly available information automatically, as soon as a benchmark improvement has been approved
- Work hosted on the SINBAD development platform (on-premise NEA Data Bank GitLab), with issue tracking

Prerequisites	**Maturity Level**				
	1	2	3	4	5
Re-distribution rights for experimental data and documentation has been obtained	☒				
Experiment documentation according to Section 1 of Evaluation Guide (SINBAD TRG, 2019[3])					
• Description of the measurement facility		☒			
• Description of each measurement configuration		☒			
• Description of materials		☒			
• Description of radiation sources		☒			
• Measurement of input and output variables		☒			
• Data in basic machine-readable format (e.g. CSV)		☒			
Evaluation of measurement data (Section 2 of Evaluation Guide (SINBAD TRG, 2019[3]))					
• Evaluation of measurement configuration			☒		
• Evaluation of radiation source			☒		
• Evaluation of the measured data			☒		
• Provision of computation models which have been used for evaluations			☒		
• Sensitivity and uncertainty analysis (including provision of computation models)				☒	
• Data in hierarchical machine readable data format (e.g. HDF5)					☒
Geometry as CAD model					☒
Benchmark model (Section 3 of Evaluation Guide (SINBAD TRG, 2019[3]))				☒	
Sample case results and input files for related computational models (Section 4 of Evaluation Guide (SINBAD TRG, 2019[3]))				☒	
Provision of automatic pre- & post-processing chain for the benchmark models					☒

News on SINBAD – on-going Task Force

Chair: T. Miller (USA) – Secretariat O. Buss



- Important future goals
  - Acquire new entries (starting at Level 1 = re-distribution rights for experimental data and documentation provided)
  - Develop requirements and provide technical capabilities for Level 5
    - Standard machine readable data formats
    - Ideally up to and including CAD, with agreed standards and translation data/tools
  - Support of Continuous Integration (CI) / Continuous Testing (CT)
    - Acquire scripts for automatic work chains (pre- and post-processing)
    - NEA GitLab has (moderate) on-site CI cluster implemented ➔ creative ideas highly welcome!
  - Continuous optimisation of process

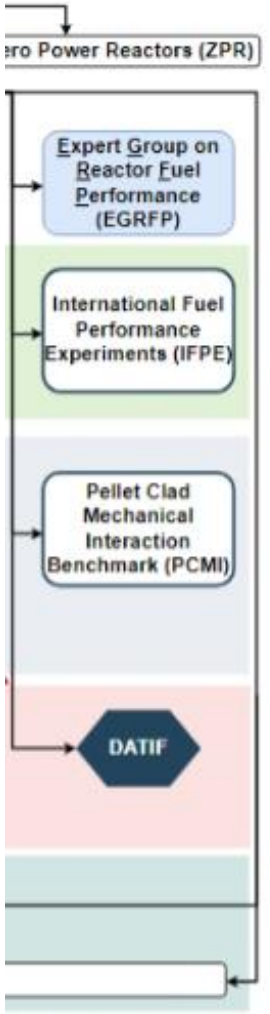
NEA/IAEA International Fuel Performance Experiments (IFPE), NEA's DATabase for IFPE (DATIF)

EGRFP Chair: G. Rossiter (UK) – Secretariat M. Bales

- IFPE contains 1452 rods/samples from various sources encompassing BWR, CAGR, PHWR, PWR, and VVER

- DATIF (=relational database for IFPE) is scheduled to be bundled with IFPE as a first step of the release, and will be dispatched along with the IFPE collection by the NEA Data Bank Computer Program Services

www.oecd-nea.org/ifpe
www.oecd-nea.org/datif



Short recap

- The Data Bank is implementing new ways of working to support collaboration within the NEA, to provide better services and to improve engagement with our service recipients
  - First implementation examples with software (e.g. SERPENT 2.2), database (e.g. SINBAD TF), data (JEFF hackathon)
  - Content on benchmark/handbooks to be developed
- Reforms to the JEFF project to strengthen the project-based elements of the group, increase engagement across the NEA and stimulate technical contributions
- Education and training activities strengthen with new platforms available and the launch of new training events
  - On-going survey https://forms.office.com/r/iE2kjWQHqr
- Close co-operation between STCs and MBDAV and with their national networks will strongly support the new, integrated services combining data, code and benchmark activities
- All the NEA is possible thanks to external contributions and involvement – your contributions, including feedback, is highly valuable!

Thank you for your attention

alice.dufresne@oecd-nea.org
programs@oecd-nea.org

NEA member countries

The NEA's current membership consists of 34 countries in Europe, North America and the Asia-Pacific region. Together they account for approximately 82% of the world's installed nuclear capacity.

Nuclear Data Sensitivity Tool (NDaST)

Benchmarks (Sensitivities) → Nuclear Data (% Change or Covariance) → Integral Results

Select / load benchmarks

Sensitivities (S) & C/E data

DICE

IDAT

Personal

Numerical Benchmarks

New Implementing handling of JSON SG45 format

Database of over 4000 Sensitivity Data Files

User Input Perturbation (P)

isotope/reaction/energy cross section

AND /OR

Covariance data via JANIS (C)

Built in processed data for major libraries

Load personal (coverx)

M energy groups (fixed)

JANIS MF33: ENDF/B-VII.1 = 2138 files, JEFF-3.2 = 5688 files JENDL-4.0 = 2155 files TENDL-2013 = 77811 files, SCALE6.2

S*P

Δk_{eff} for selected cases

C/E output plot grouped by criteria

S*C*S^T

$U_{C(XS)}$ for selected cases

Additional uncertainty on output plot grouped by criteria

Matrix plot showing individual contribution to $U_{C(XS)}$ by isotope-reaction

New Implementing command line for implementation in pipelines

www.oecd-nea.org/ndast

JEFF stakeholder follow-up

- Stakeholder engagement recognised as essential for nuclear data development – the bridge between physics and end-users
- Efforts such as the NEA High-Priority Request List and similar efforts elsewhere help guide/prioritise efforts but require engagement to populate
- 2019 meeting yielded many insights and put people in contact for the first time
- MBDAV has requested to launch another international stakeholder meeting with co-operation across NEA programmes