The Modern Nuclear Energy Agency Data Bank: An Integrated Hub for Code and Data Development and Validation

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Head of the Data Bank

IAEA ONCORE meeting

20-24 June 2022
Politecnico di Milano

Data Bank work areas

The Data Bank is a 'Centre of Reference' for computer codes, nuclear data, benchmarks, training and knowledge preservation – formed in 1977 as part of the OECD Nuclear Energy Agency.

Mission evolves over time covering 3 main work areas:

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.

Nuclear Energy Agency

OECD members (38)

Chile, Colombia, Costa Rica, Estonia
Israel, Latvia, Lithuania, New Zealand

NEA members (34)

Australia, Canada*, Iceland, Ireland
Luxembourg, United States*

*Dedicated agreement with the DB for computer programs

NEA DB members (28)

Austria, Belgium, Czech Rep, Denmark
Finland, France, Germany, Greece
Hungary, Italy, Japan, Korea
Mexico, Netherlands, Norway, Poland
Portugal, Slovak Rep., Slovenia, Spain
Sweden, Switzerland, Turkey, UK
Argentina, Bulgaria, Romania, Russia**

** member (suspended) pursuant to a decision of the OECD Council

NEA's Agreement with the IAEA provides IAEA Members that are not OECD members access to some DB codes

Argentina, Bulgaria, Romania and Russia are not member countries to the OECD (June 2022)

Technology implementation

1. **New GitLab instance with on-site Harbor, Docker and NEA CI cluster** and launched in March 2022 that supports CPS and NDS activities. This is a long-term solution following pilot projects with limited functionality.
2. **New Canvas LMS (eLearning)** launched in April 2022 with first course pilot on the open source OpenMC code. A new blockchain-based credentialing system with social media integration is in progress **(Accredible).**
3. **SharePoint MyNEA** to replace oecd-nea.org/download was launched in May 2022 (where much NEA content is now stored). This will be used for official meetings and is being considered for DB restricted file content management.
4. **More in progress** including a public SharePoint system for machine-readable data storage (coming Q3 2022) and static-site-generated content for advertisement of NEA GitLab and associated system content.

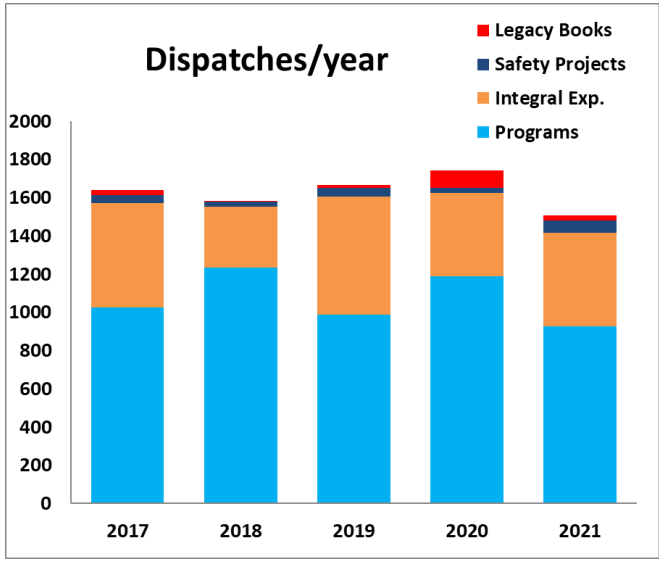
Data Bank Computer Program Service (CPS)

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

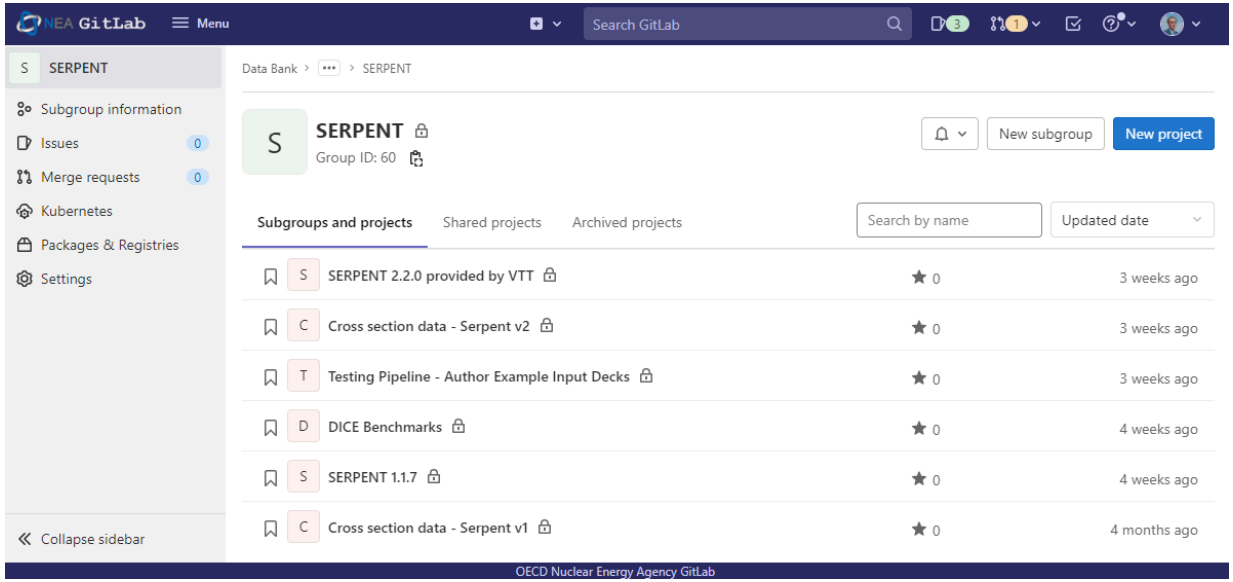


Year	Programs	Integral Exp.	Safety Proj.	Legacy Books	Total
2017	1024 (62%)	547 (33%)	41 (3%)	28 (2%)	1640
2018	1234 (78%)	317 (20%)	27 (2%)	5 (0%)	1583
2019	986 (59%)	618 (37%)	47 (3%)	15 (1%)	1666
2020	1188 (68%)	438 (25%)	26 (1%)	90 (5%)	1742
2021	928 (62%)	488 (32%)	66 (4%)	24 (2%)	1506

CPS 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 quality checks 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 – distribution starting in May 2022 of Serpent-2 (VTT, Finland) Monte-Carlo code



CPS new working methods (II)

Update docker/ubuntu-20/Dockerfile
ADIGUN Babatunde authored 1 week ago

Dockerfile 307 Bytes

```
FROM registry.oecd-nea.org/infra/docker-registry/ubuntu:20.04-NEA

RUN apt-get --yes update && \
    apt-get --yes upgrade && \
    apt-get --yes install make gfortran git build-essential gcc zip python python3.7 python3

#RUN mkdir -p /home/serpent/src
COPY . /home/serpent/
RUN cd /home/serpent/src; make
```

- Reproducible container configuration, automatically processed @NEA GitLab
- Images built, stored, and available for internal pipelines or distribution w/Harbor

```
Cloning into 'cross-section-data'...
warning: redirecting to http://git.oecd-nea.org/databank/cps/serpent/cross-section-data.git/
Updating files:  60% (3/5)
Updating files:  80% (4/5)
Updating files: 100% (5/5)
Updating files: 100% (5/5), done.
[32;1m$ bash data-unpack.sh[0;m
Unzipping data libraries to location data/
Archive:  endfb68.zip
   creating: endfb68/acedata/
  inflating: endfb68/acedata/1001ENDF68.ace
  inflating: endfb68/acedata/100255JEF311.ace
```

- Nuclear data directly integrated at image level for testing, distribution and end-use
- Complete testing environment for devs of code/data with real-time feedback

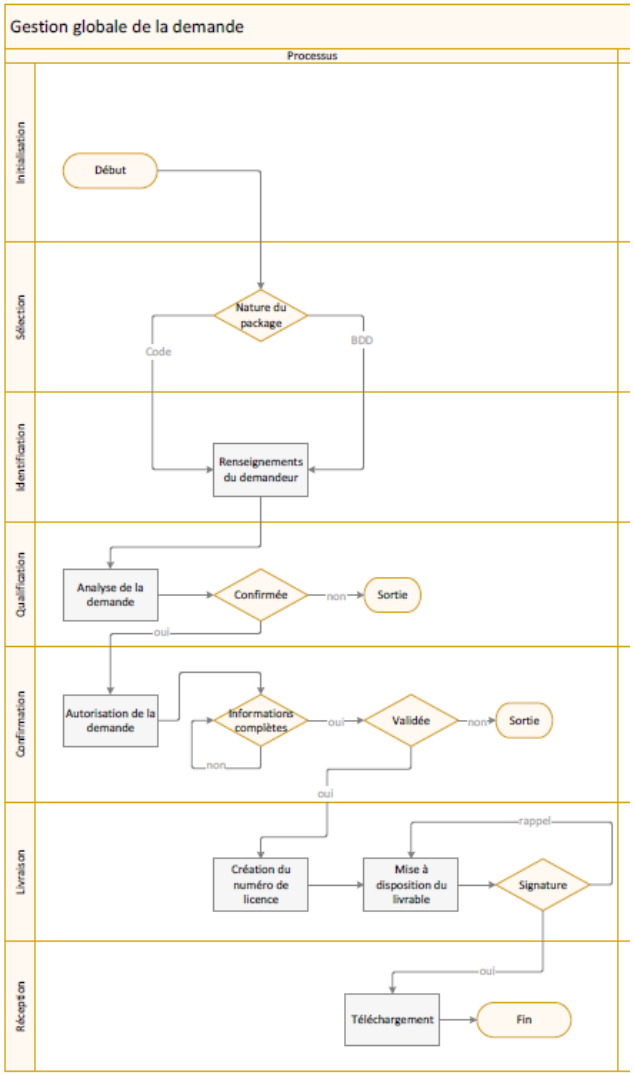
```
orevaluepair.o suggestnexttime.o suggestnexttimeinterval.o sumdivcompositions.o sumprivatedata.o sumprivateres.o su
al.o surfacesrc.o surfacevol.o swapitems.o swapuniverses.o symboliclu.o symmetryboundary.o systemstat.o targetveloc
p.o testhisvbreak.o testparam.o testsurface.o teststlgeometry.o teststlsolids.o testunisym.o testvaluepair.o testxs
valstr.o timercpuval.o timerval.o timestamp.o timestr.o tobank.o tocommonque.o tolimbo.o torusdis.o toque.o tostack
de.o transportcycle.o transportcorrection.o trapz.o trapzreal.o truncate.o tta.o ttb.o ttachain.o ttaloop.o ufsfact
updatefinixpower.o updateifcdensmax.o updateifctempminmax.o updatemicrodens.o updatermxwgt.o uresdilumicroxs.o ures
valuepairidx.o valuepairval.o vectornorm.o vectorprod.o virtgcucolflags.o volumesmc.o vrcycle.o walkeralias.o warn
ritedepfile.o writedepletioninterface.o writedynsrc.o writefinixinputfile.o writetetmeshtogeo.o writefinixifc.o wri
eumshtostl.o writewwmesh.o wwdis.o wwimportance.o wwinsrc.o xsplotter.o zaitoiso.o zdis.o zonecount.o -lm -o sss2
Serpent 2 Compiled OK.
Removing intermediate container 3ffb7617377b
 ---> 41708acf46a8
Successfully built 41708acf46a8
Successfully tagged registry.oecd-nea.org/cps/serpent/serpent-2.2.0:ubuntu-20_gfortran
$ docker push $CI_HARBOR_REGISTRY/$CI_HARBOR_REGISTRY_PROJECT/$NEW_PROJECT_PATH:ubuntu-20_gfortran
The push refers to repository [registry.oecd-nea.org/cps/serpent/serpent-2.2.0]
```

```
 _                    .-=-.          .-=-.          .-==-.
{ }      __        .' O o '.      .' O o '.      /  -<' )--<
{ }    .' O'.     / o .-. O \    / o .-. O \    /  .---`
{ }   / .-. o\   /O  /   \  o\  /O  /   \  o\  /O /
 \ `-` /   \ O`-'o  /     \  O`-'o  /     \  O`-`o /
  `-.-`     '.____.'       `._____.'       `.____.'
Serpent 2.2
A Continuous-energy Monte Carlo Reactor Physics Burnup Calculation Code
 - Version 2.2.0 (May 5, 2022) -- Contact: serpent@vtt.fi
 - Reference: J. Leppanen, et al. "The Serpent Monte Carlo code: Status,
              development and applications in 2013." Ann. Nucl. Energy,
              82 (2015) 142-150.
 - Compiled May 18 2022 16:00:37
 - MPI Parallel calculation mode not available
 - OpenMP Parallel calculation mode not available
 - Geometry and mesh plotting not available
```

CPS system renewal

Modernisation of CPS distribution tools

- To develop an integrated platform that better serves the needs of users and facilitate CPS internal work
  - To handle adaptable workflows with various options, to cover all encountered cases, IE, benchmarks, SAF packages, IAEA requests, etc.
  - To create user accounts including their request history
  - To generate more secure download links, based on a dedicated infrastructure
  - To introduce automated reporting workflows
- Current status: **pre-specification**, formalisation of workflows and requirements
- Next steps: contracts for specification and architecture studies in late 2022

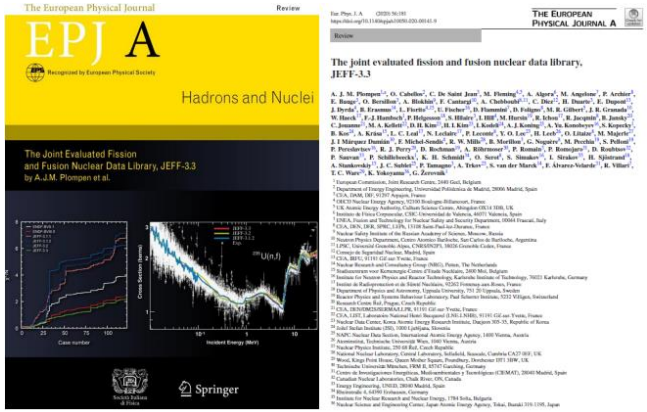


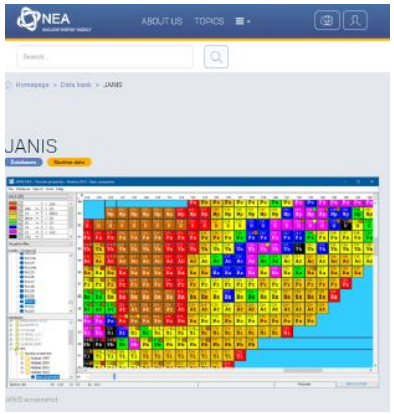
Data Bank Nuclear Data Service (NDS)

- 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.





Nuclear data: JEFF reform

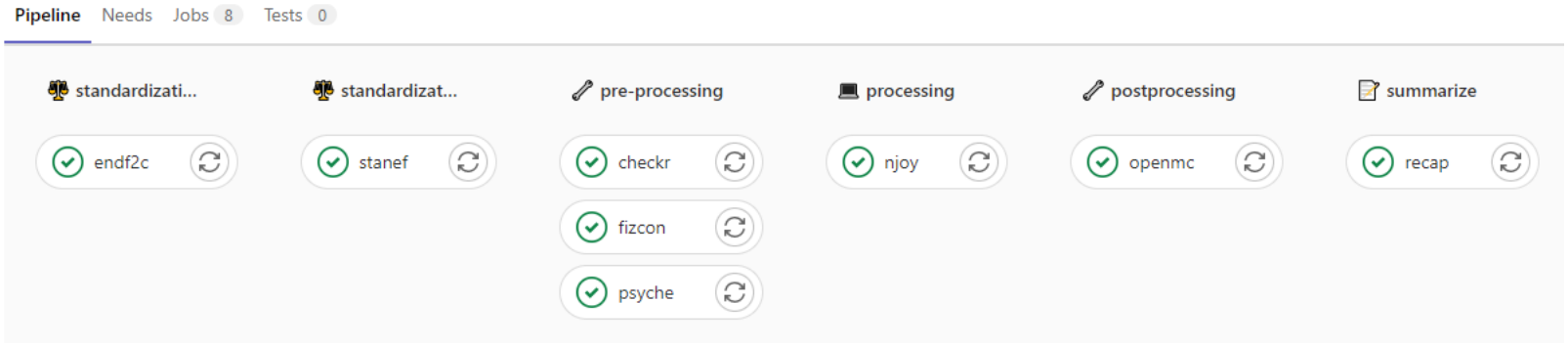
- 12 newly established technical groups and a project review group for the Co-ordination Group
- Significant increase in the engagement and quality of the content of the meeting
- Technical session Chairs brought energy and insight, working closely with NEA Secretariat to create technical agendas
- 3x – 6x the technical presentations compared with last 3 years of meetings
- 16 specific and Actions were raised, 13 Decisions were taken [NEA/MBDAV/DOC(2021)16]

JEFF technical engagement

- 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	TBD
9.	Dedicated iron evaluation and testing	TBD
10.	Pipeline HACKATHON	TBD Sep 2022

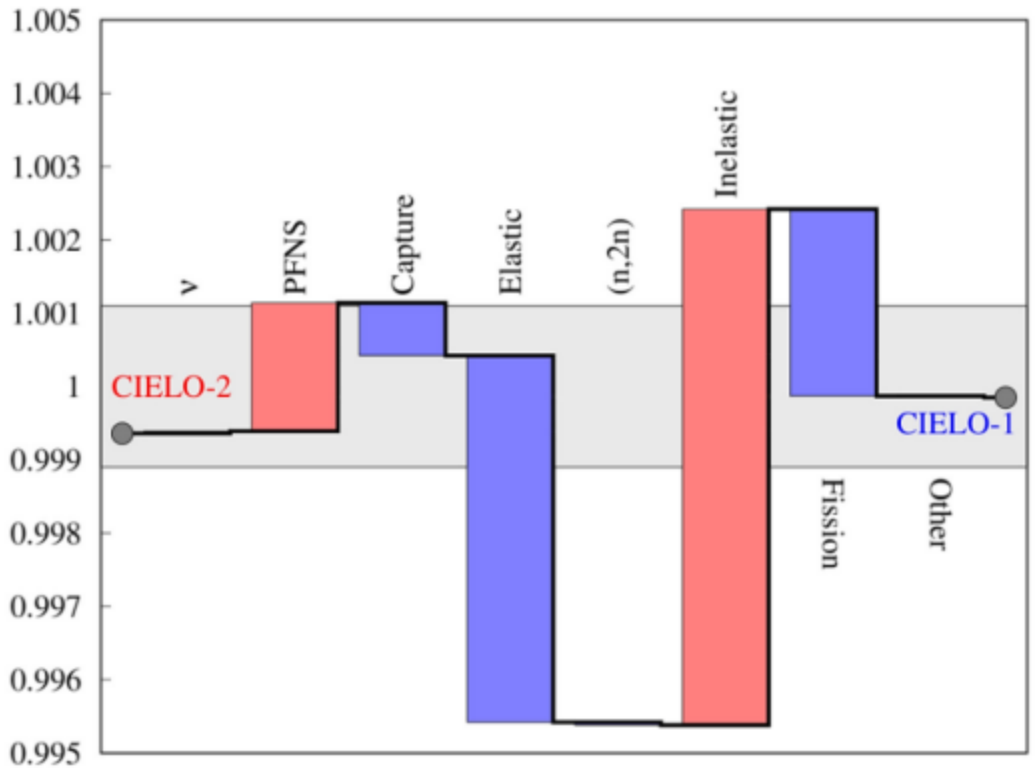
- And adoption of GitLab-based workflows to manage the project, test the data in real time and directly integrate it with computer codes within the CPS catalogue (see previous slides)



Nuclear data adjustment

- Nuclear data take differential measurements + semi-empirical models as the starting position
- Integral measurements are essential to giving accurate results for real applications
- Adjustment occurs explicitly (e.g. GLLS) or implicitly within eval.
- There is no unique solution – **posteriors are application specific**

Figure 5. Waterfall of the differences between the CIELO-2 (left) and CIELO-1 (right) evaluations in the simulation of the Jezebel bare plutonium sphere benchmark (PMF1)

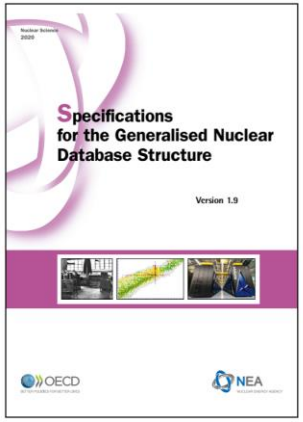


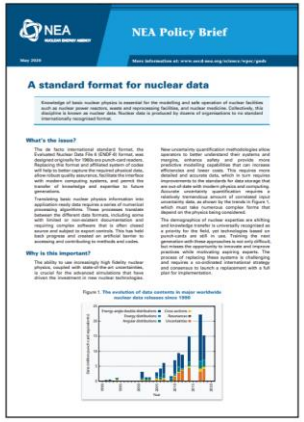
GNDS (new ENDF) project

Objective: To create and maintain a modern international standard for the storage of nuclear data 'GNDS'

- EG-GNDS formed as an official body to finalise the first specifications and create a process for continual updates – ***first publication 2020***
- ***NEW specifications 2.0 approved in May 2022 meeting!***
- ***APIs and processing codes already out and open source (e.g. FUDGE, GIDI, more)***
- Webinar hosted by NEA on GNDS-1.9, Chaired by NEA DG Magwood and Dr David Brown with international panel

https://youtu.be/h9Byrkxr8LE





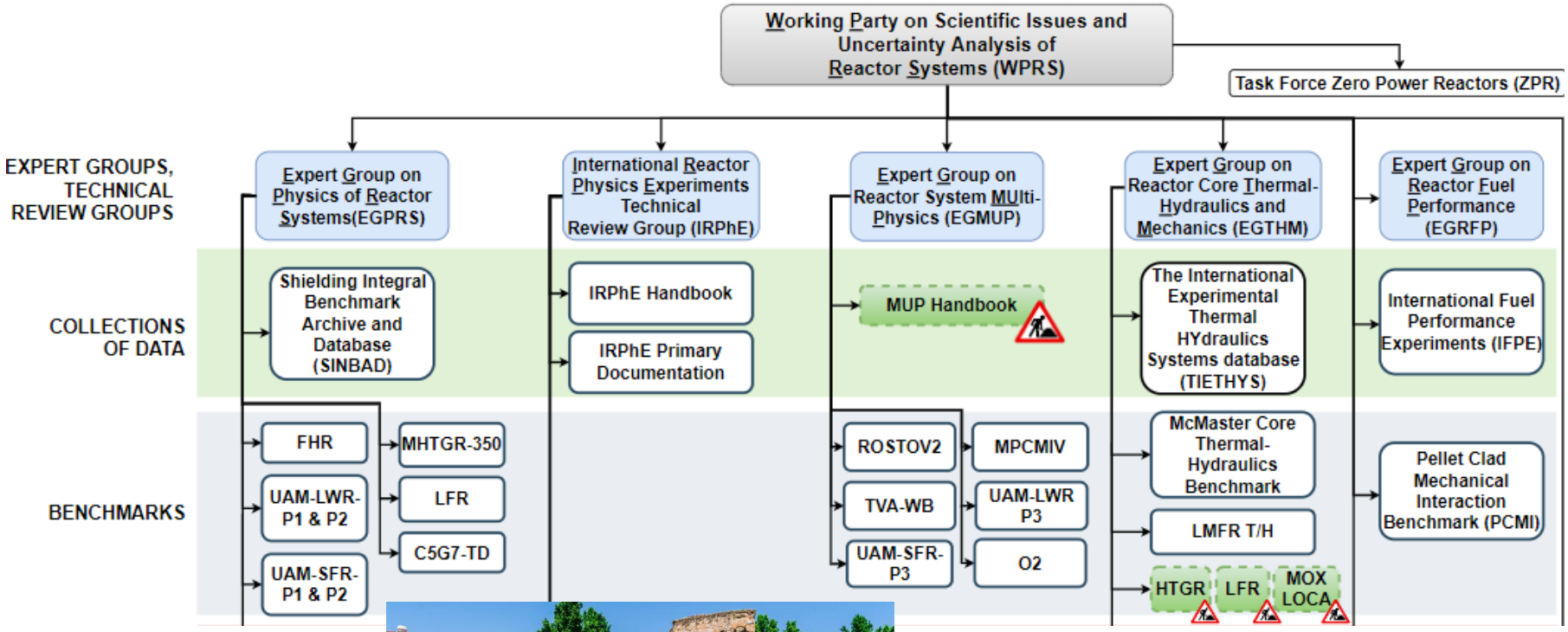
GNDS version 1.9 (first publication) May 2020

ISBN 978-92-6490-197-1

342 page detailed technical specifications

With a policy brief for high-level/general audience

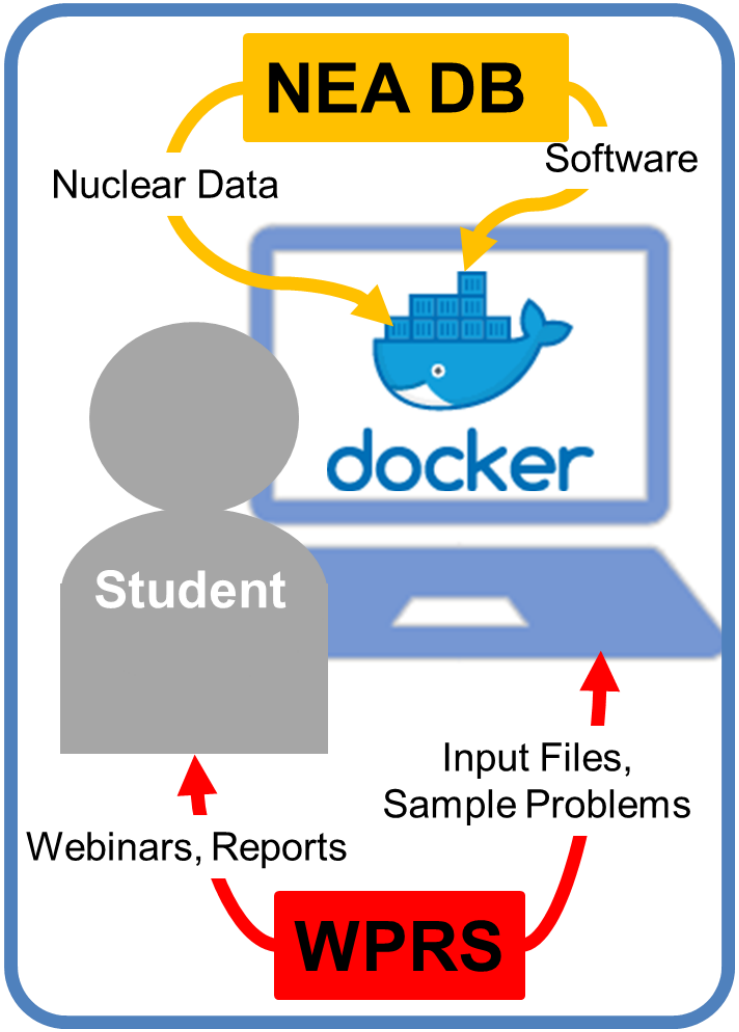
NEA / NSC benchmark activities



NEA/NSC
WPRS-2022 benchmarks
@CEA Cadarache

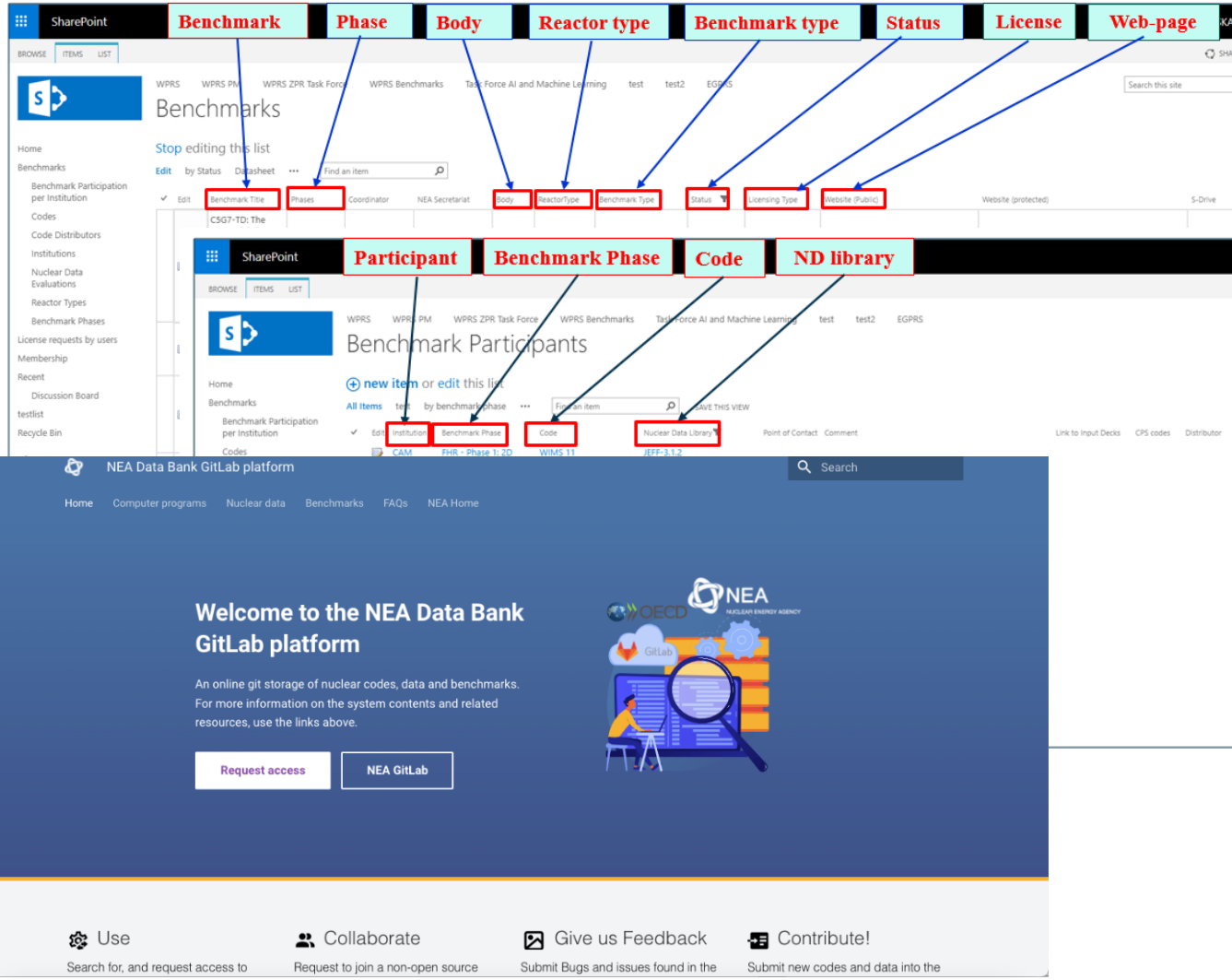
Benchmarks – collaboration

- New code and data containerised environments are natural support for education and training activities
- Collaboration between NSC and DB on benchmarks to standardise and simplify distribution and access rules
- Newly acquired code packages and upcoming releases through DB will help support this initiative
- **Area for engagement with members** to help expand access for more software packages to improve the catalogue of potential simulation systems
- **Pilot project will be selected in coming months** with WPRS to demonstrate educational benchmark outreach
- Categorisation and UI/X for non-delegate users required to effectively filter for relevant information



Benchmarks – categorisation effort

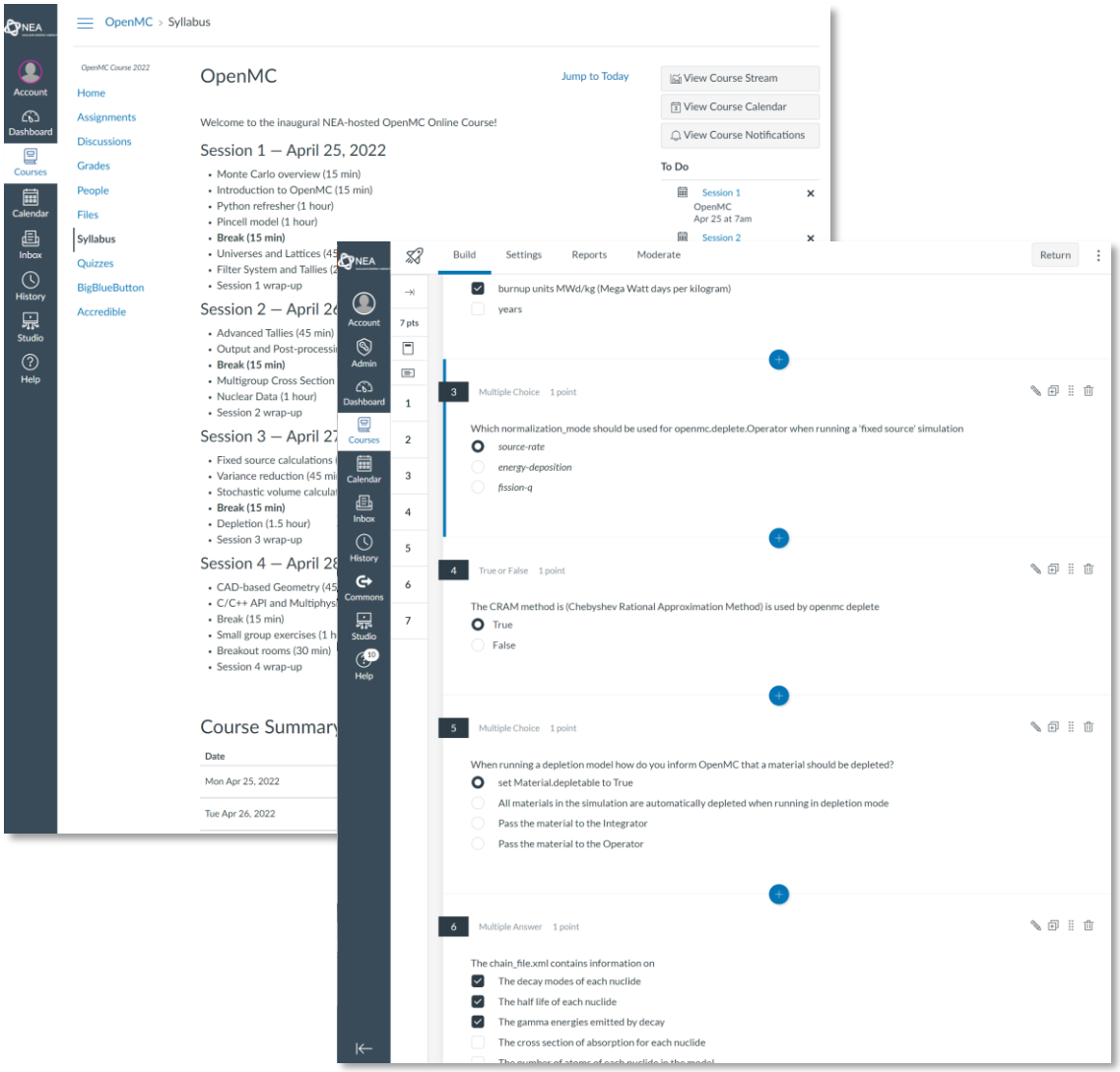
- NSC and DB Secretariat have worked to classify benchmark activities
- Subset of content will be used for public-facing GitLab pages content to direct users to relevant materials
- Users will be able to access codes, data, benchmarks and be informed of relevant training activities
- **Benchmark expert engagement key** to content population



eLearning background

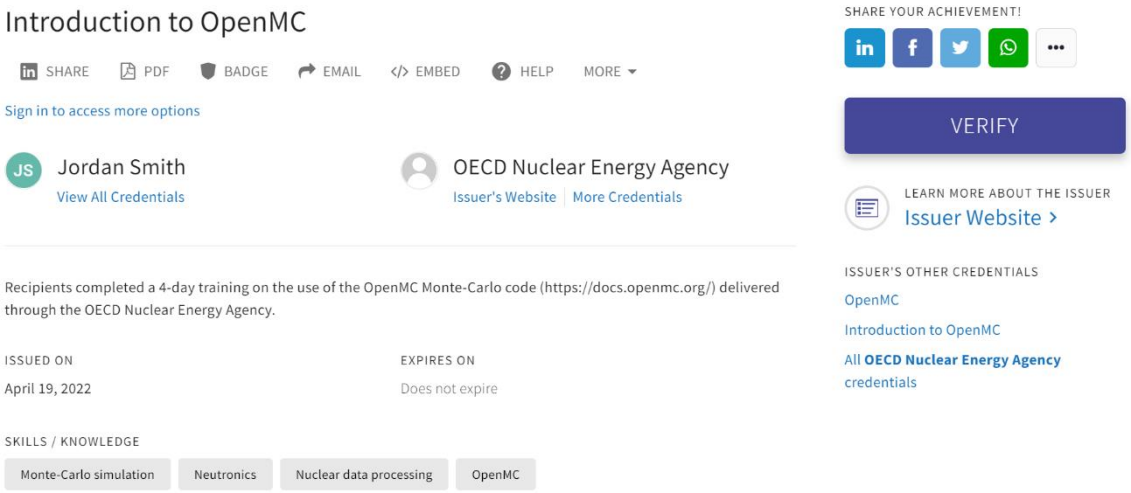
- Data Bank trainings have been held virtually for the past two years due to the pandemic
- In-person trainings are resuming this summer, **some CPS trainings will be held online even in the future, and in-person courses will continue to contain digital elements**
- With the new digital landscape, there has been a **need to find better long-term solutions**
- NEA launched a new eLearning system with Canvas LMS in April 2022
- First pilot with **OpenMC** open source Monte-Carlo code

- **Easy implementation** even with short time frame (tool available less than two weeks before the course)
- Course naturally defined with module and syllabus tools to structure content
- The course took place on Zoom and all course content was accessed through Canvas
- Assignments and reviews conducted in the system significantly increased engagement
- **Positive feedback** from participants and teachers – who have asked for a repeat

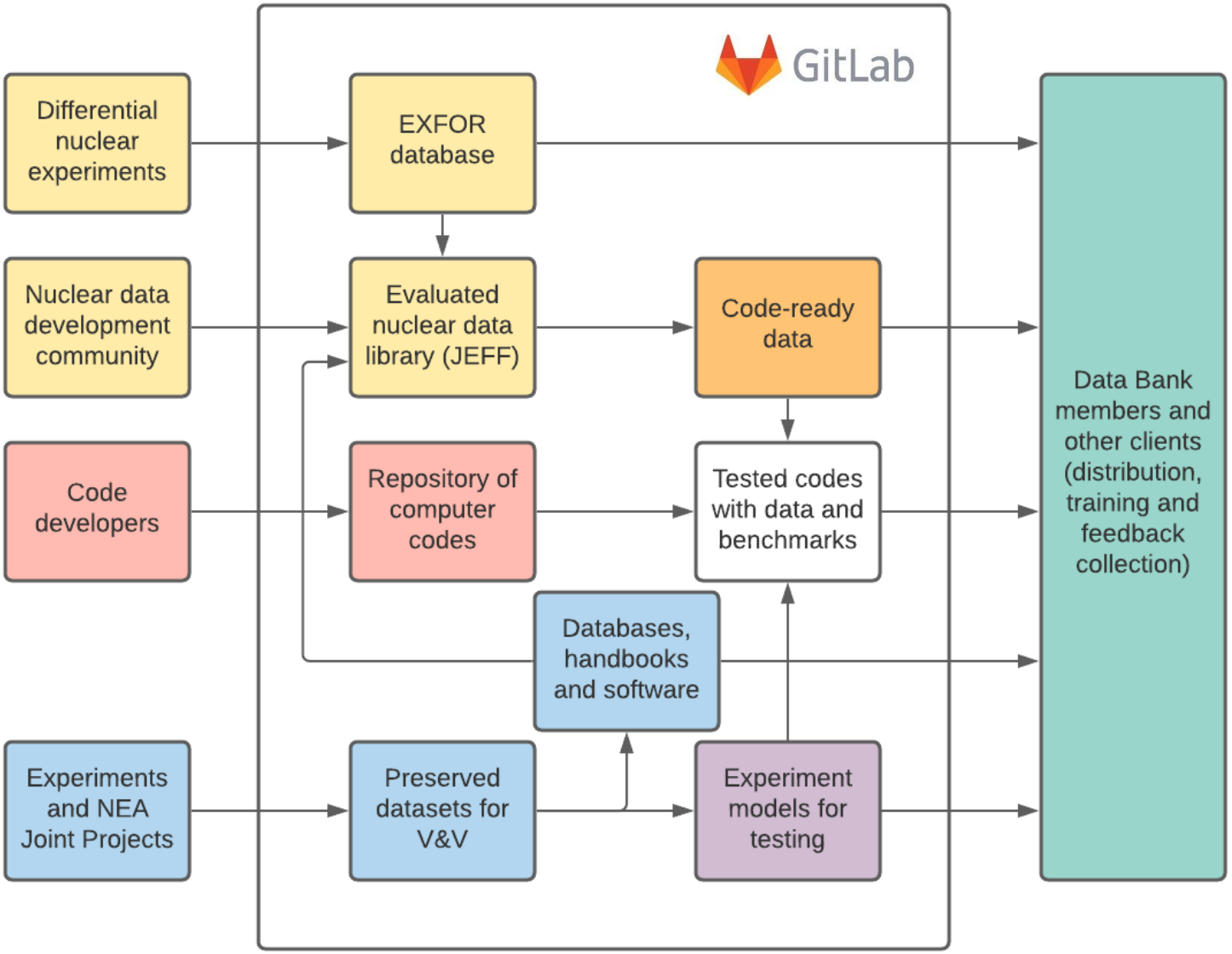


Nuclear Energy Agency

- (Pilot) Accredible credential system will issue digital badges for social media
- Badges sharable e.g. with LinkedIn with blockchain verification
- NEA catalogue of courses and certificates
- Links to course, NEA and provider (if requested) to provide cachet, marketing and publicity
- Describing outcomes and exercises increases value
- Assignments and pass/fail integrated into Canvas before issuing credentials
- Available in June 2022 (planned)



Nuclear Energy Agency



Brief recap

1. **Implementing new technology systems** and transition projects onto these systems, to support cross-unit and division interaction and to better engage with our service recipients.

2. **Modernisation and improvement of CPS practices** to support integration of services previously focused on distribution.

3. **Reforms to the JEFF project** to strengthen the project-based elements of the group, increase engagement across the NEA and stimulate technical contributions.

4. **Engagement across data+code** developer communities with the **NEA benchmarks** to save, disseminate and leverage for training the 'code related content' for benchmarks

5. **Support education and training through eLearning** to complement the return to physical training events and better engage remote participants with mature, mixed-content systems.

Thank you for your attention

All NEA publications and institutional documentation available at
www.oecd-nea.org