Euratom 2019-2020 Grant agreement No 900018

Design, population and exploitation of a database on radiation embrittlement of reactor pressure vessels: the ENTENTE H2020/EURATOM project

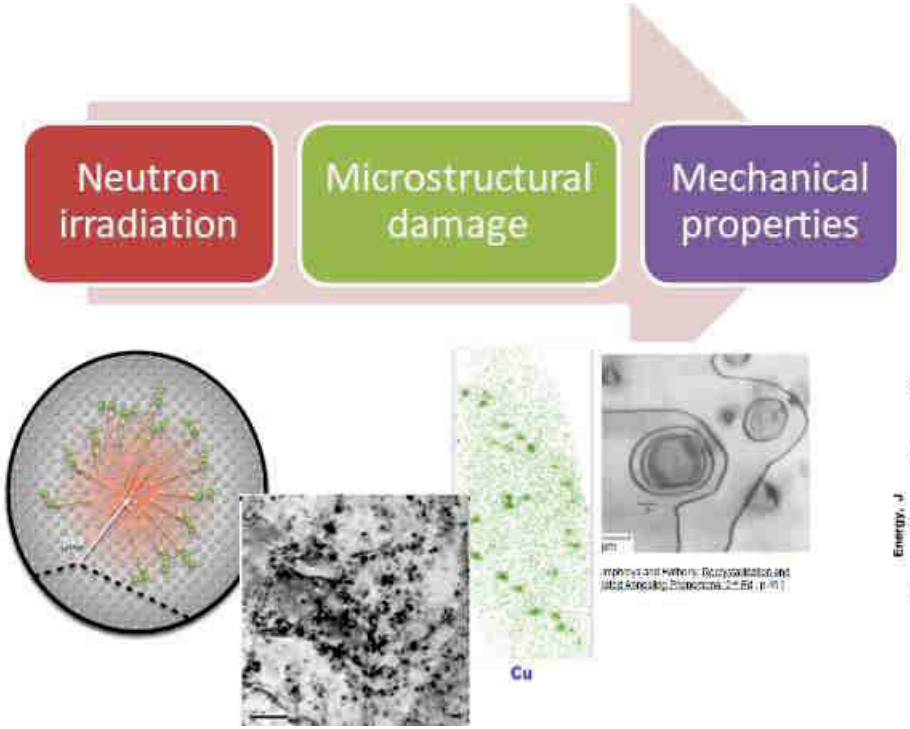
Project Coordinator: Marta Serrano (CIEMAT)

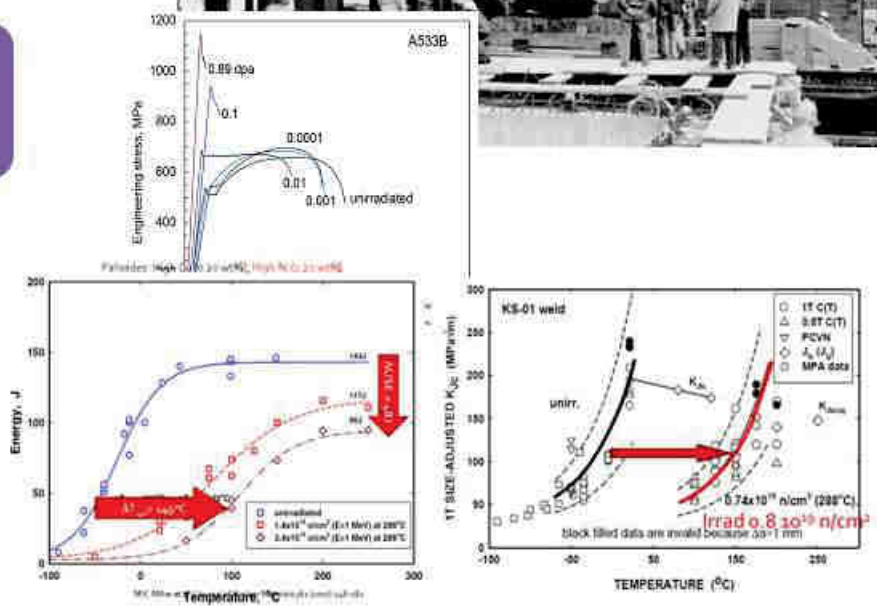
WP leaders: Julien Sanahuja (EDF), Christian Robertson (CEA), Matti Lindross (VTT)

The problem

- Neutron embrittlement of the reactor pressure vessel

- RPV Dimensions (1000 MWe)
  - Height =10-20 m
  - Wall thickness = 15-30 cm
  - Inner diameter= 4 - 5 m
- Operational conditions
  - 12.5 - 15.5 MPa for PWRs and 7-8 MPa for BWRs.
  - The maximum coolant temperature is about 330°C.
  - Radiation environment





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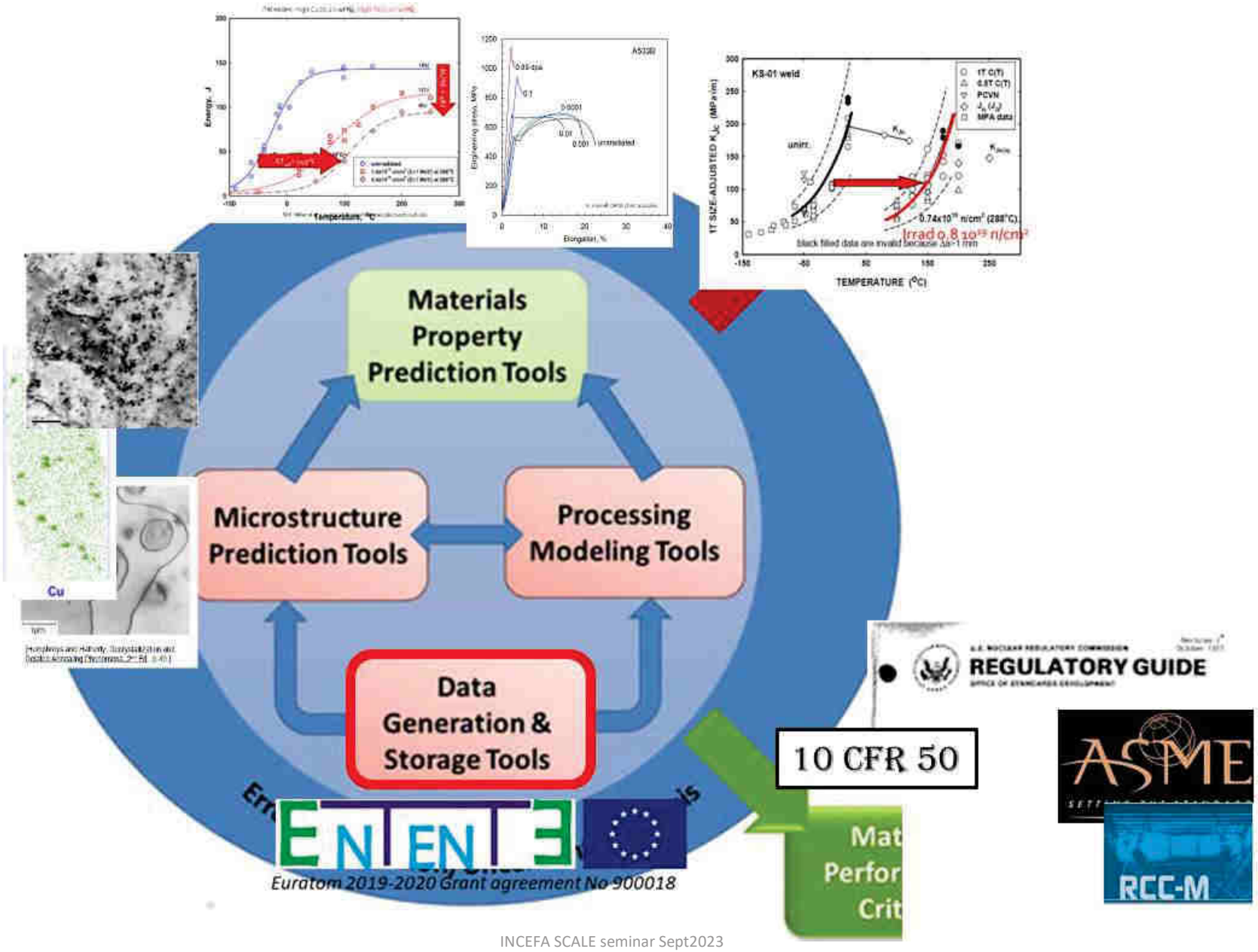
The approach: “Materials informatic”

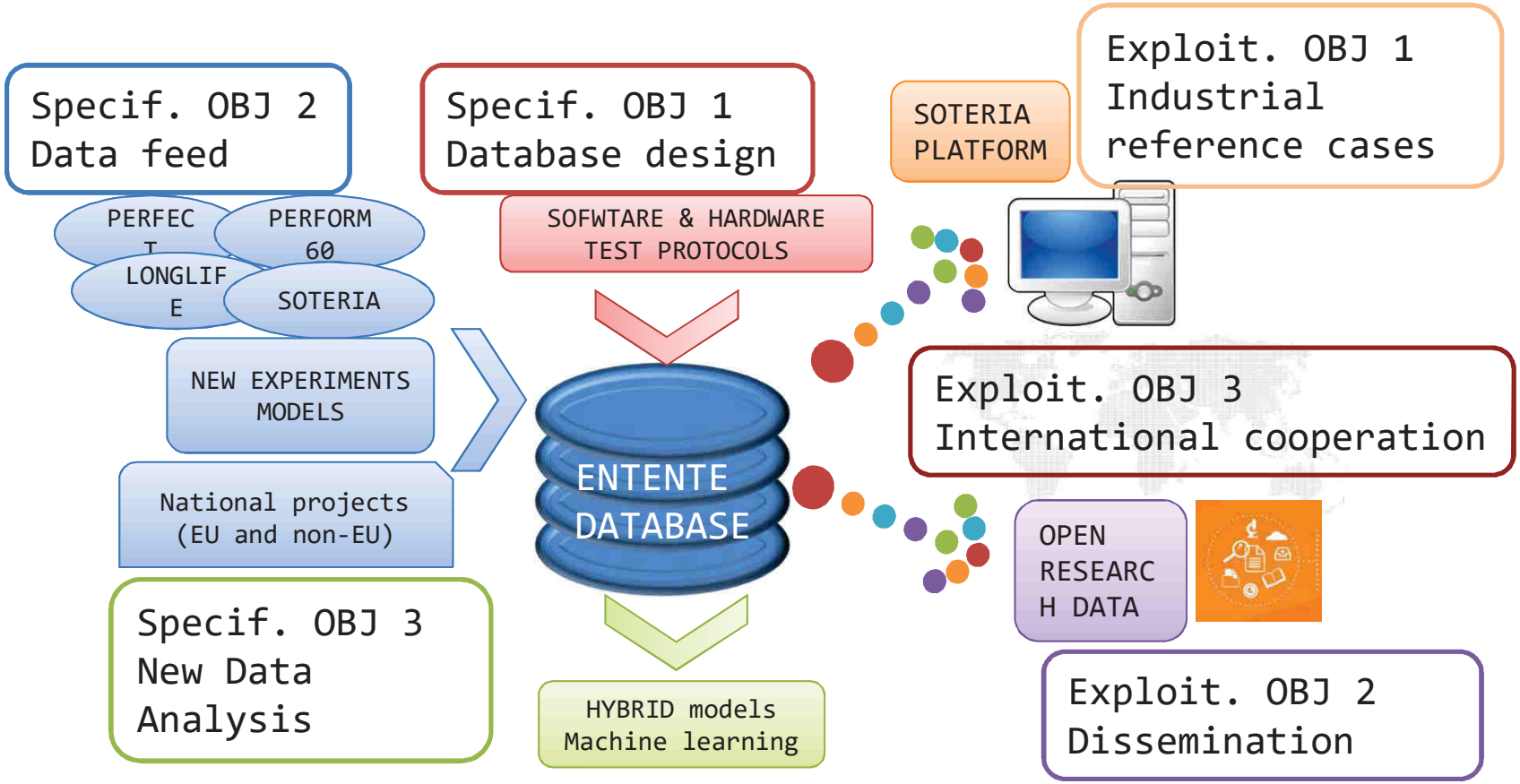


ENTENTE

- ENTENTE "European Database for Multiscale Modelling of Radiation Damage" aims to design a **new European experimental/modelling materials database** to collect and store highly-relevant data on **radiation damage of Reactor Pressure Vessel (RPV) steels**
  - EURATOM Call NFRP-2019-2020-01.Ageing phenomena of components and structures and operational issues
- **Specific objectives**
  - Design and maintain a unique experimental/modelling database for model validation and calibration
  - Collect previous data and enrich the database with microstructural and mechanical data on neutron irradiated RPV materials to fill gaps
  - Development of advanced models based on data analytics/mining and previous knowledge
- **Exploitation objectives**
  - Improve the SOTERIA Platform
  - Encourage the dissemination of results
  - Foster International collaboration

EURATOM-H2020 Grant agreement nº 900018 (Sept 2020-Aug. 2024)

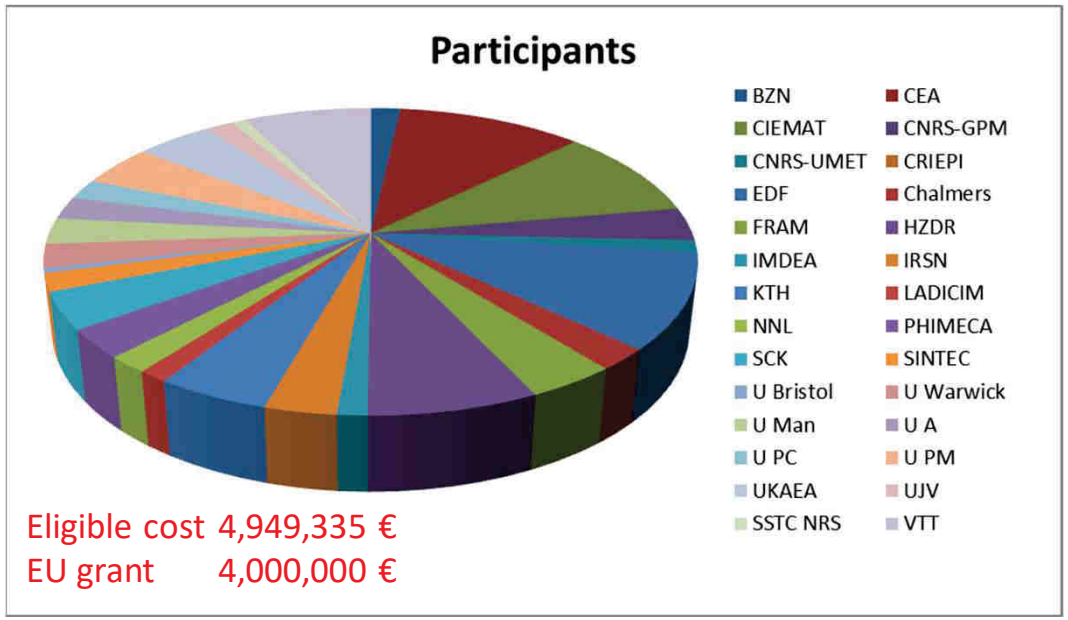
ENTENTE - Objectives



The overall objective of the ENTENTE project is to design a unique experimental/modelling database to store the results on radiation embrittlement of reactor pressure vessel steel produced within this project and along different EURATOM funded projects

ENTENTE Consortium

- 27 partners
  - Industrial partners (EDF, CRIEPI, FRA-G, UJV, NNL);
  - R&D centres (CIEMAT, BZN, CEA, HZDR, IMDEA, SCK•CEN, CCFE); Universities (CNRS, CHALM, KTH, UC, UBRIS, UWAR, UMAN, UA, UPC, UPM)
  - SME (SINTEC, PHIMECA), as well as TSO (VTT, SSTC NRS, IRSN).
- 12 countries: Spain, France, UK, Germany, Finland, Sweden, Belgium, Italy, Hungary, Czech Republic, **Ukraine and Japan.**



ENTENTE DataBase

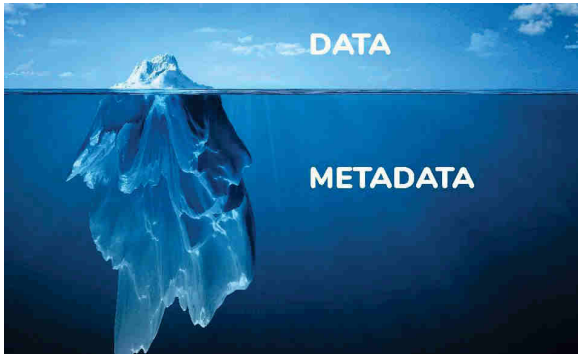
- Key challenges -> **Data Base architecture**
  - Definition of the database specifications according to end user cases and development of a database or repository that provides persistence, conservation and **easy access** to both experiments and models data and metadata.
    - In particular, the necessary structure of database will be defined according to end user needs, by exploring first relational SQL databases, such as PostgreSQL, and then, noSQL databases, with less overhead, although with weakest semantics.
  - Development of appropriate interfaces to data and metadata, reusing state-of-the-art recommendations (e.g., DCAT-AP [DCAT-AP]), which guarantee an efficient data flow.
  - **Long term maintenance – CIEMAT/NEA DataBank**

ONTOLOGY

DCAT-AP Interface

Relational SQL

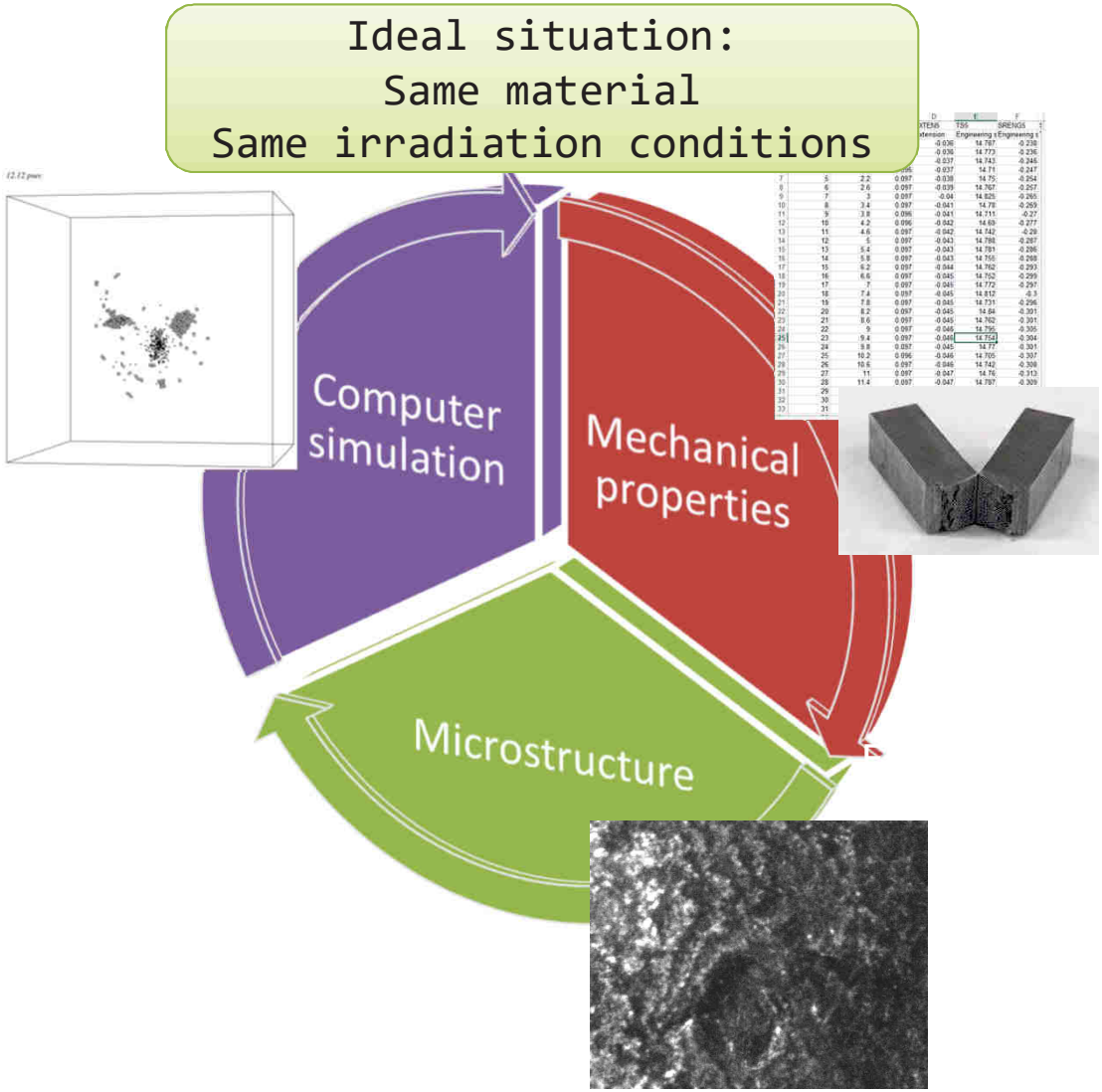
Metadata



ENTENTE DataBase

- Key challenges -> **rescue of old data**

- Data produced from different partners within different agreements
- Stored in personal computers
- Experimental and/or modelling gaps
- Data pedigree



ENTENTE DataBase

- Key challenges -> **define data formats**
  - Proper homogenization to bridge the meso- to macro-scale and efficient data extraction techniques
  - **Interoperability with other materials database**

European Materials Modelling Council (EMMC)

European Materials Characterisation Council (EMCC)

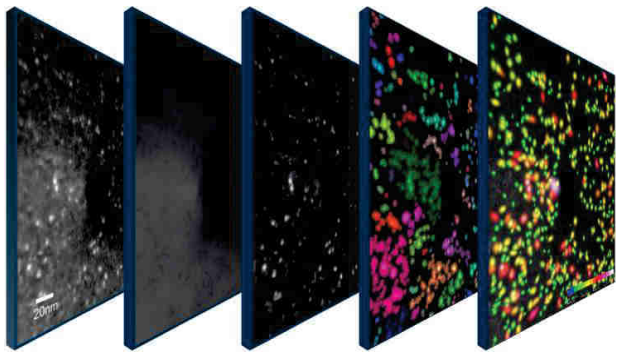
International Atomic Energy Agency
Atomic Molecular Data Services
Provided by the Nuclear Data Section

NEA Nuclear Energy Agency

CascadeDB

Data Format and data quality committees

CIEMAT	Coordinator
SCK•CEN, HZDR, CIEMAT, EDF, VTT, CCFE	Microstructure data formats: Small Angle Neutron Scattering (SANS), Electron Back Scattering Diffraction (EBSD), Positron annihilation spectroscopy (PAS), Atom Probe Tomography (APT), Scanning and transmission electron microscopy (SEM and TEM),
FRA-G, CIEMAT, CRIEPI	Mechanical property data formats: mechanical testing such as tensile tests, Charpy Impact test, fracture toughness tests (R&D and surveillance capsules results)
EDF, CNRS, KTH	Modelling data formats: underlying data from models used in microstructure modelling (Atomistic Kinetic Monte Carlo, Object Kinetic Monte Carlo, Cluster Dynamics and Rate Theory) to describe migration of point defects and point defect clusters (migration and dissociation energy barriers, diffusion prefactors, etc.) and thermodynamics of the system (cohesive model, capillary law, etc.)



D.R. Mason

ENTENTE DataBase

- Key challenges -> **data collection**
  - Definition of data stewardship workflows that describe the processing of data and the generation of metadata, automatically connecting the execution of experiments with the process of storing and archiving the output data in the database

Best practices protocols
Re-education of scientist

Implementation

WP1 (CIEMAT)- Management

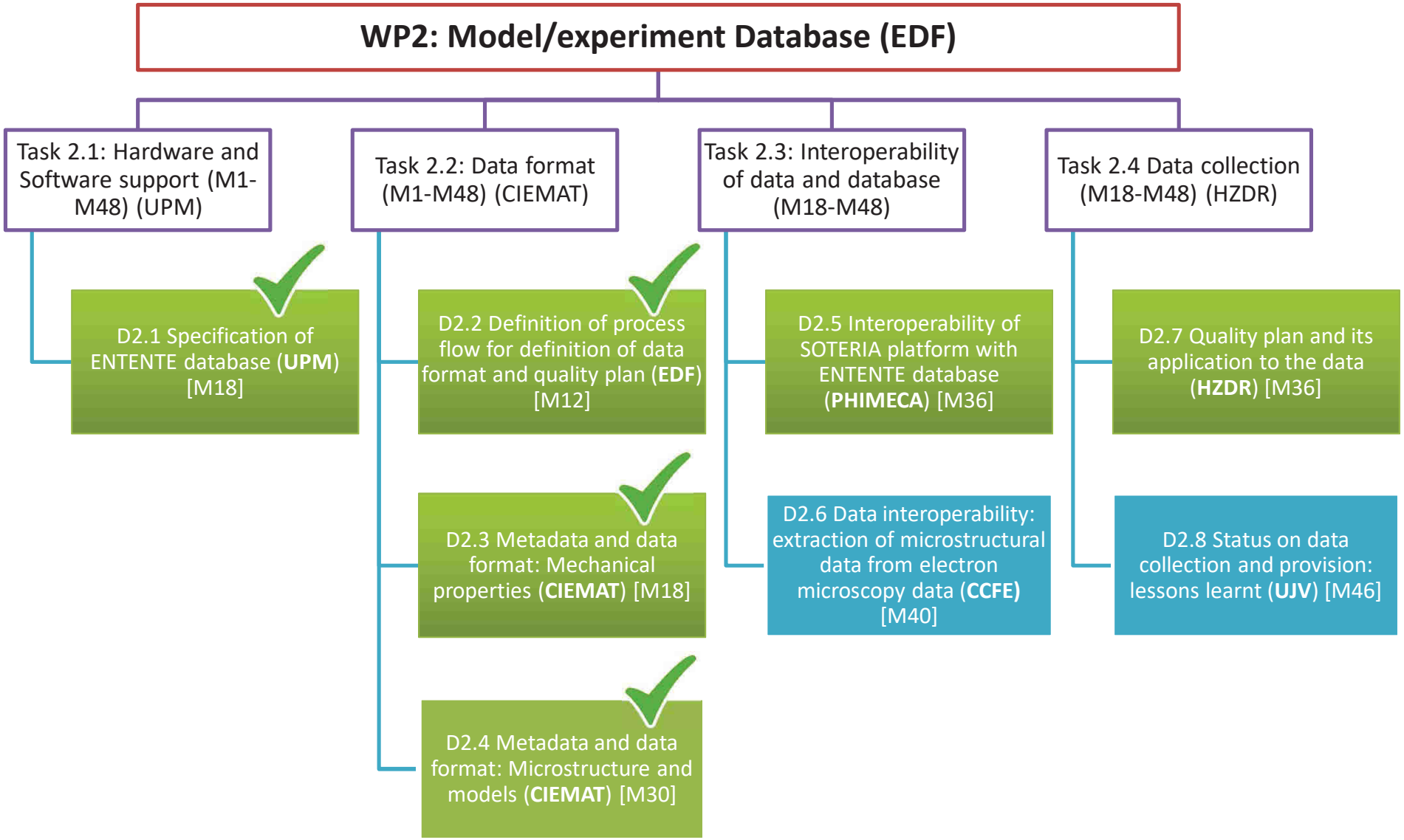
WP5 (CIEMAT) - Dissemination, exploitation and training

WP2 (EDF) - Model/experiment database
Database design
Data collection
SOTERIA PLATFORM

WP3 (CEA) - Generation of experiment/modelling data
Dedicated experiments and models
Atomistic -> Fracture

WP4 (VTT) - Accelerated model and analysis approaches
ICME approaches
Artificial networks and Machine learning.
Hybrid atomistic

WP2 (EDF) - Model/experiment database

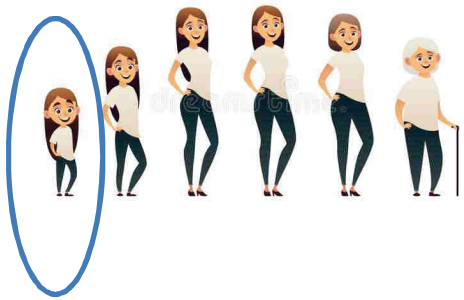


First steps

Mechanical properties

Microstructure

Models



Data formats

- Committes

Structure

- PLOTTER&REAP

Integration

- SOTERIA Platform

WP2 (EDF) - Model/experiment database

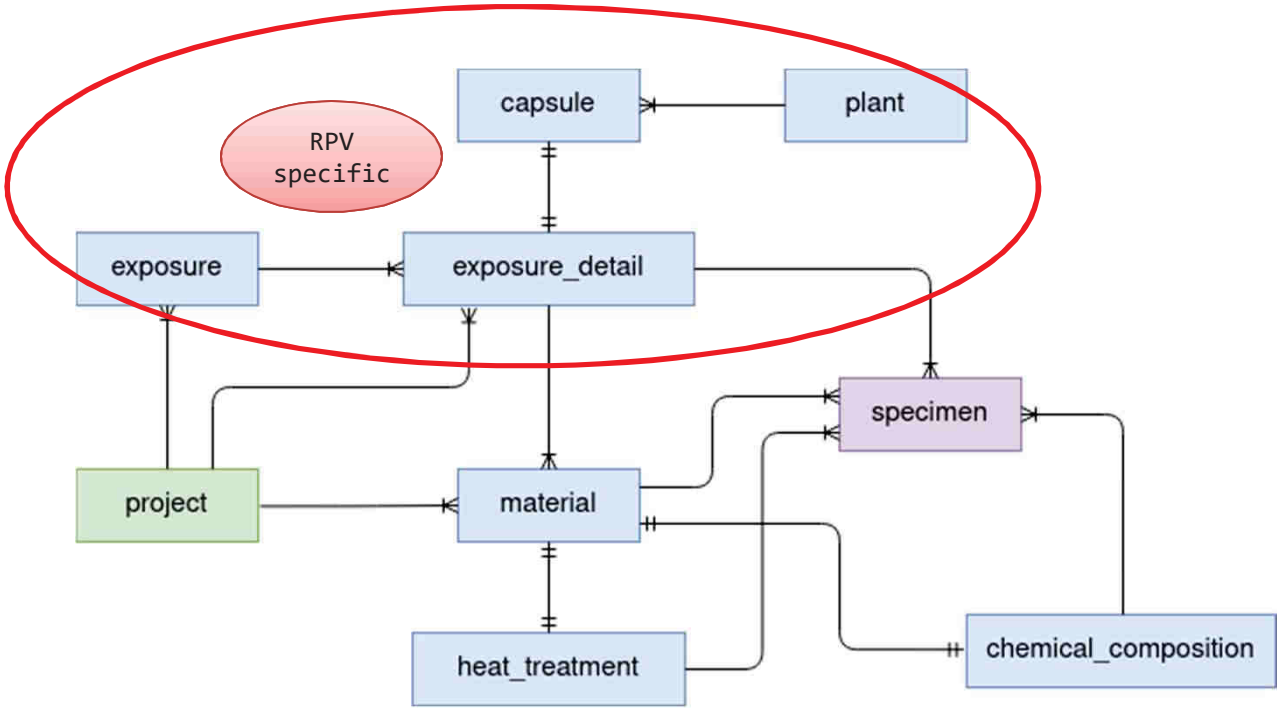
Data Formats

9 data committees of experts have been formed, one for each mechanical testing, microstructure examination and modelling techniques

Committee	Chair	Members
Transmission Electron Microscopy	Mercedes Hernández Mayoral (CIEMAT)	Data producers: Wade Karlsen (VTT), Grace Burke (UMAN), Paul Chekhonin (HZDR), Joven Lim (UKAEA); Frédéric Delabrouille (EDF) Data users: Lorenzo Malerba (CIEMAT), Nicolas Castin (SCK-CEN), Daniel Mason (UKAEA), Christophe Domain (EDF), Ghiath Monnet (EDF), Giovanni Bonny (SCK-CEN)
Scanning Electron Microscopy (SEM)/ Electron Backscattering Diffraction (EBSD)	Paul Chekhonin (HZDR)	Data producers: Wade Karlsen (VTT), Grace Burke (UMAN), Susana Merino (CIEMAT), Joven Lim (UKAEA) Data users: Matti Lindroos (VTT); Frédéric Delabrouille (EDF), Ghiath Monnet (EDF), Christian Robertson (CEA)
Atom Probe Tomography (APT)	Paul Styman (NNL)	Data producers: Bertrand Radiguet (CNRS), Kristina Lindgren (Chalmers) Data users: Lorenzo Malerba (CIEMAT), Nicolas Castin (SCK-CEN), Christophe Domain (EDF), Gilles Adjanor (EDF), Patrick Todeschini (EDF), Ghiath Monnet (EDF); Akiyoshi Nomoto (CRIEPI)
Small Angle Neutron Scattering (SANS)	Andreas Ulbricht (HZDR)	Data-producers: Nicolas Martin (CEA) Data users: Lorenzo Malerba (CIEMAT), Nicolas Castin (SCK-CEN), Christophe Domain EDF), Gilles Adjanor (EDF)
Positron Annihilation Spectroscopy (PAS)	Giovanni Bonny (SCK-CEN)	Data-producers: Milan Konstantinovic (SCK-CEN) Data users: Lorenzo Malerba (CIEMAT), Christophe Domain (EDF), Pär Olsson (KTH)
Mechanical properties	Hieronymus Hein (FRA-G)	Data-producers: Marta Serrano & Rebeca Hernández (CIEMAT), Eberhard Altstadt (HZDR), Miloš Kytka (UJV); Data users: Patrick Todeschini (EDF), Ghiath Monnet (EDF), Nicolas Castin (SCK-CEN); Mark Kirk (CRIEPI), Milan Brumovsky (UJV), Jean-Philippe Mathieu (EDF)
Atomic scale models (DFT, MD, …), thermodynamics and kinetics data	Pär Olsson (KTH)	Data-producers/users James Kermode (Warwick U.), Napoleón Anento (UPC), Giovanni Bonny (SCK-CEN), Charlotte Becquart (CNRS), Christophe Domain (EDF), Julien Vidal (EDF), Gilles Adjanor (EDF)
Microstructure evolution models (O/AKMC, …)	Charlotte Becquart (CNRS)	Data-producers/users: Daniel Mason (UKAEA), María José Caturla (UA), Lorenzo Malerba (CIEMAT), Christophe Domain (EDF), Gilles Adjanor (EDF), Nicolas Castin (SCK-CEN), Giovanni Bonny (SCK-CEN)
Mechanical modelling data (single and poly crystals)	Ghiath Monnet (EDF)	Data-producers/users: Matti Lindroos (VTT), Roxane Marull (CEA), Nicolas Castin (SCK-CEN), Jean-Philippe Mathieu (EDF)

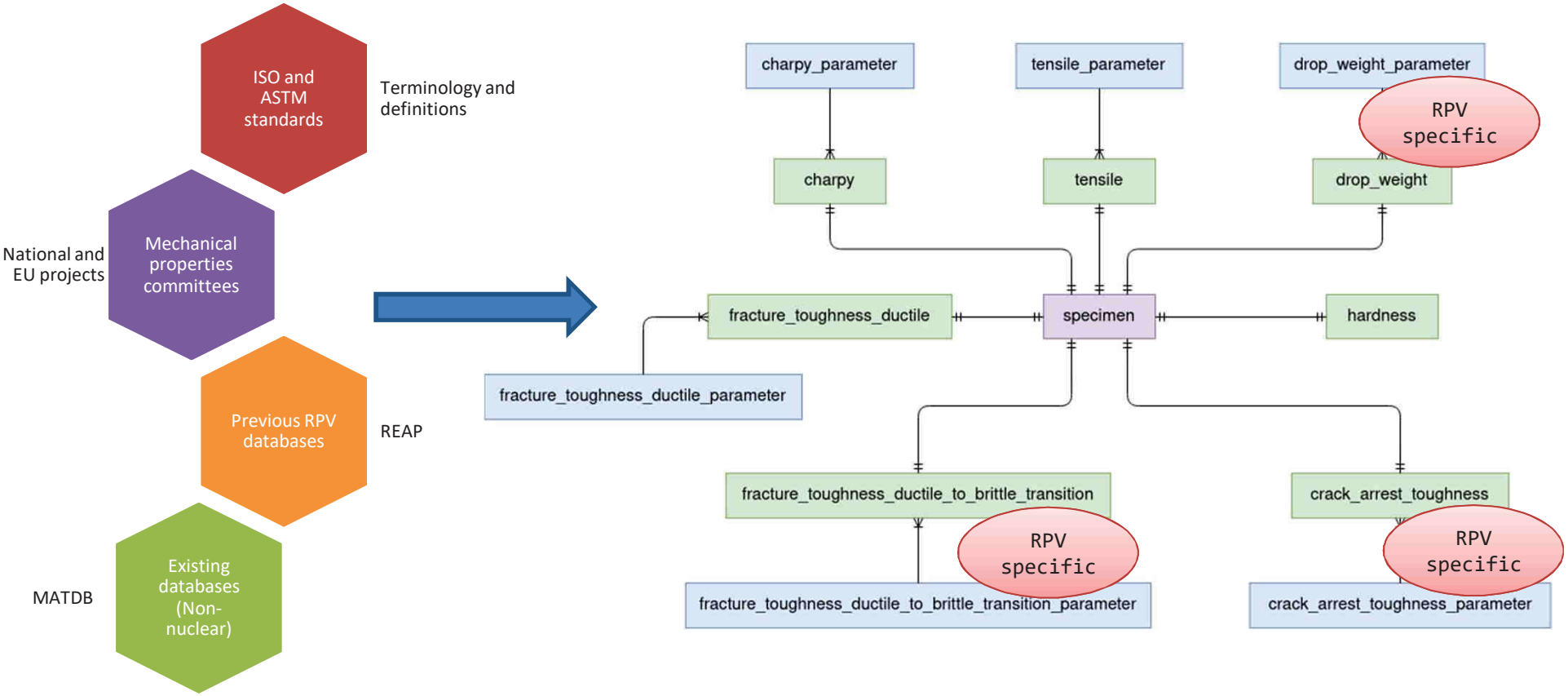
WP2 (EDF) - Model/experiment database

- The ENTENTE database is composed of a **high-level part,** which acts as the core that connects to other modules.
- These modules refer to specific techniques (e.g., mechanical properties, SEM or APT).
- This modular structure facilitates data ingestion, and its later exploitation, as different techniques can be treated independently, but they all share a common high-level layer.



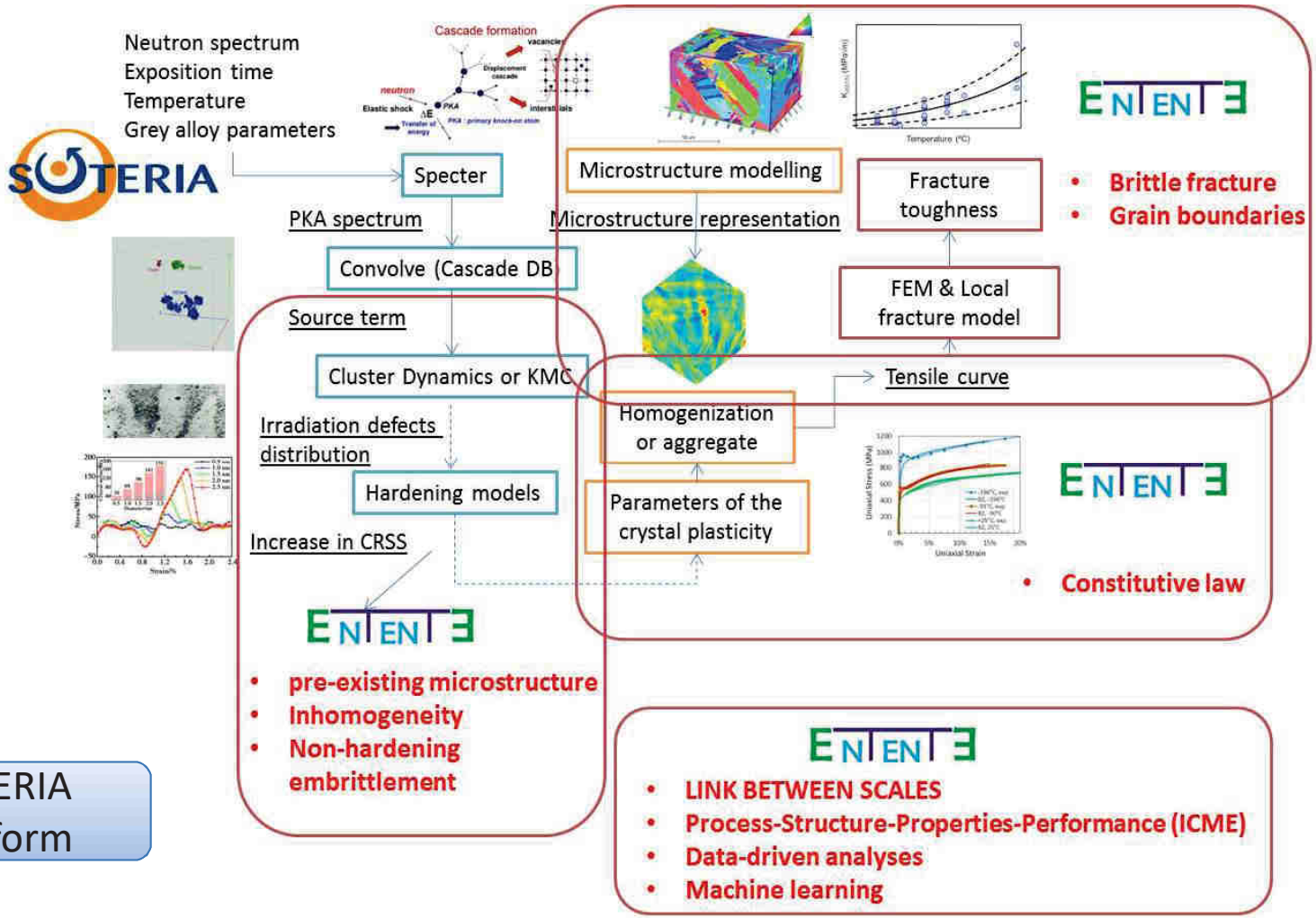
WP2 (EDF) - Model/experiment database

Mechanical properties data base already defined



WP2 (EDF) - Model/experiment database

- Virtual machine ready (incl. Windows version)



SOTERIA Platform

WP3 (CEA) - Generation of experiment/modelling data

WP3: Generation of experimental and modelling data on dose-dependent RPV steel embrittlement (CEA)

- Task 3.1: Material Supply: un-irradiated and irradiated RPV materials and model alloys (M1-M30) (FRA-G)
  - D3.1 Supply of un-irradiated and irradiated material for microstructural examinations (FRA-G) [M6]
- Task 3.2: Microstructural examinations in RPV steels and model alloys (M1-M48) (HZDR)
  - D3.2 Characterisation of un-irradiated microstructures and test matrix for irradiated materials (HZDR) [M18]
  - D3.3 Influence of chemical and structural heterogeneities on the irradiation behaviour (CNRS) [M36]
- Task 3.3: Prediction of dose-dependent non-hardening embrittlement in RPV steels (M19-M48) (CEA)
  - D3.4 Prediction of grain boundary coverage and its effect on surface energy parameter (**NNL**) [M24]
  - D3.5 Non-hardening embrittlement brittle fracture modelling (**CEA**) [M36]:
  - D3.6 Non-hardening embrittlement of RPV steels (**CEA**) [M46]:
- Task 3.4: Constitutive dose-dependent stress-strain response and associated fracture models (M12-M48) (VTT
  - D3.7 Dose-dependent constitutive models for mechanical and damage response prediction in RPV steel (**UBRI**) [M36]
  - D3.8 Prediction of dose-dependent fracture response evolutions (**VTT**) [M46]

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WP3 (CEA) - Generation of experiment/modelling data

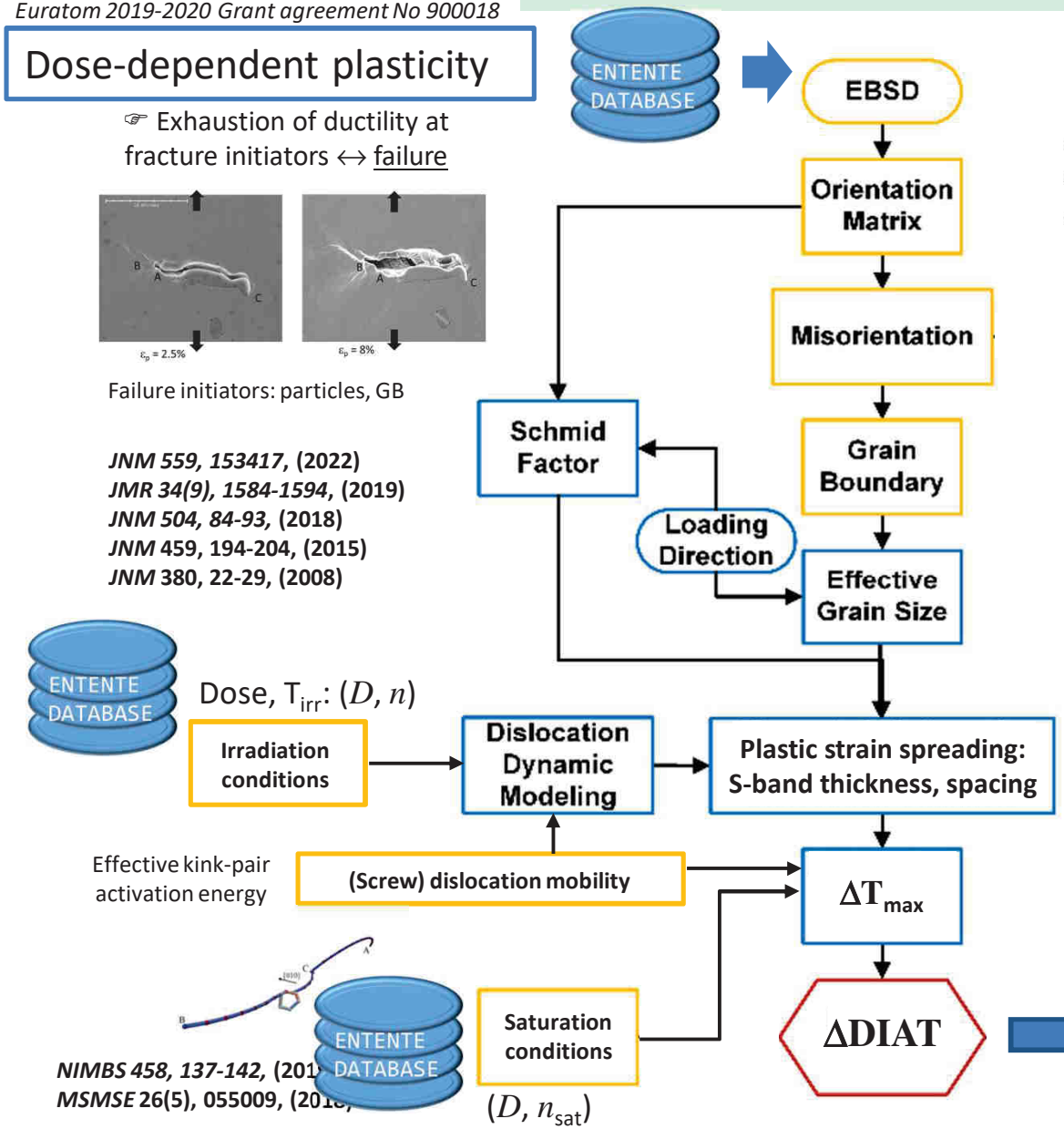
C. Robertson (CEA)

Dose-dependent plasticity

☞ Exhaustion of ductility at fracture initiators ↔ failure

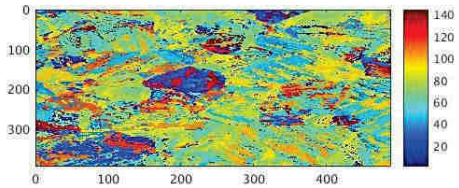
Failure initiators: particles, GB

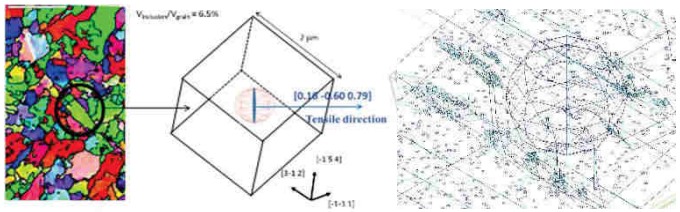
JNM 559, 153417, (2022)
JMR 34(9), 1584-1594, (2019)
JNM 504, 84-93, (2018)
JNM 459, 194-204, (2015)
JNM 380, 22-29, (2008)

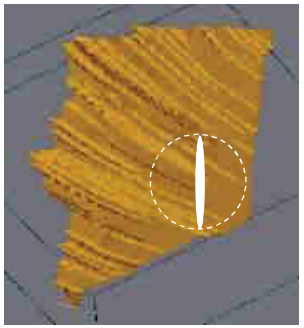


NIMBS 458, 137-142, (201
MSMSE 26(5), 055009, (201

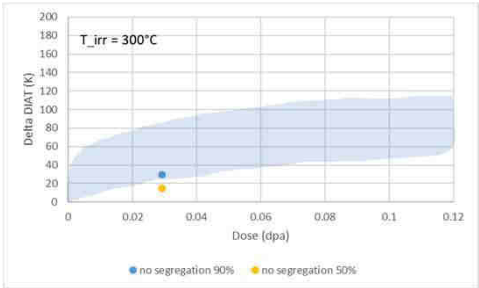
RPV steel microstructure







crack-related strain: shear bands



WP3 (CEA) - Generation of experiment/modelling data

WP4: Accelerated modelling and analysis approaches

Task 4.1: Integrated modelling approaches on LTO of RPV steels (M1-M48) (VTT,

- D4.1 Statistical analysis of stress-strain states in RPV polycrystals affecting brittle fracture by crystal plasticity simulations and validation experiments (**CEA**) [M36]
- D4.2 Irradiation spectra uncertainty impact on mechanical properties of irradiated steel (**IRSN**) [M40]
- D4.3 Integrated Computational Materials Engineering of RPV workflow for RPV steel and an assessment of LTO (**VTT**) [M46]

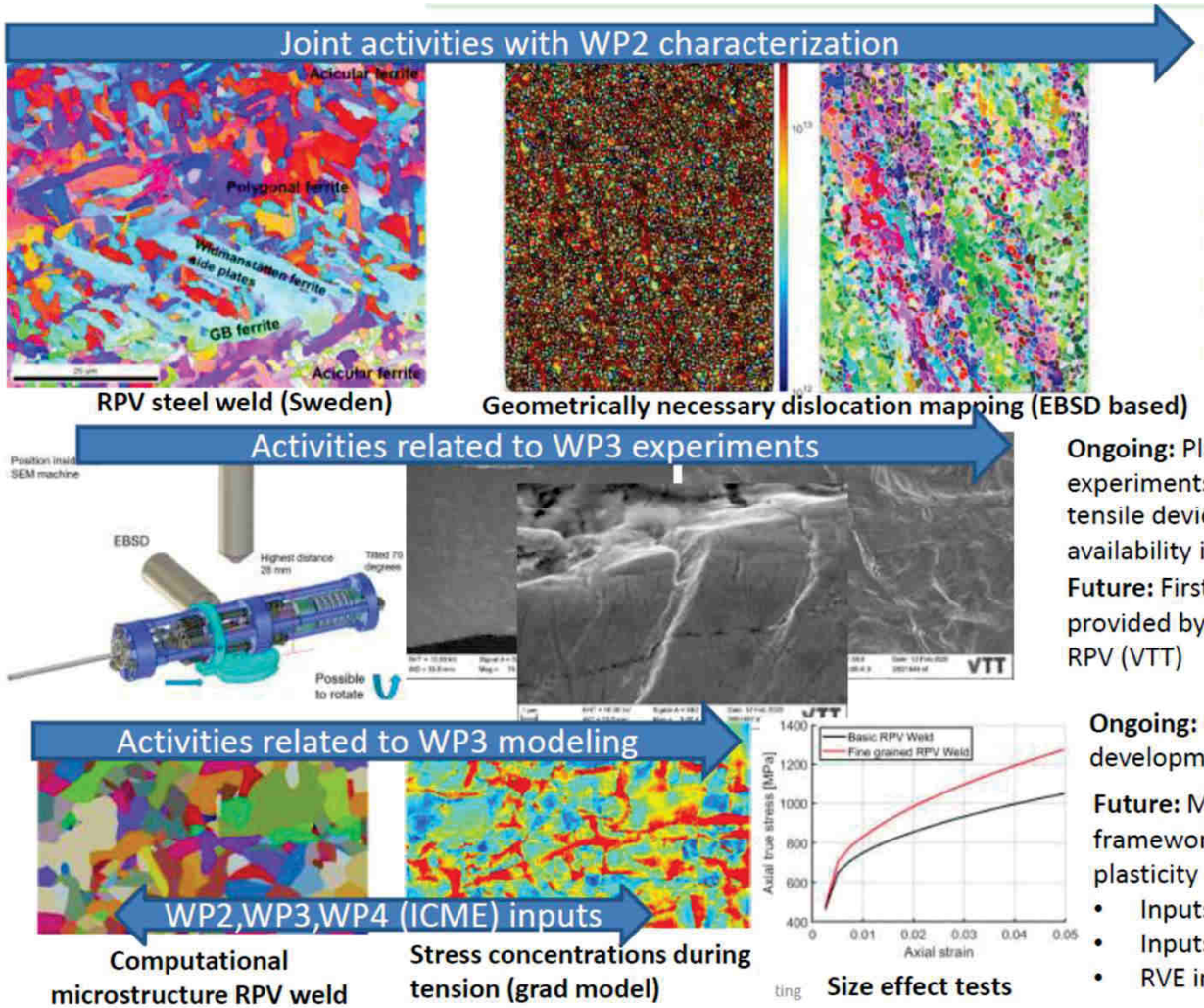
Task 4.2: Machine learning to model RPV LTO (M1-M48) (UC)

- D4.4 Machine learning (ML) as regression tool, ML in microstructure descriptors and damage identification, and development of ML algorithms for accelerated LTO estimation (**UC) M46**
- D3.3 Influence of chemical and structural heterogeneities on the irradiation behaviour (CNRS) [M36]

Task 4.3: Hybrid models on RPV embrittlement (M12-M48) (UPC)

- D4.5 Hybrid hardening models from SANS and NI experiments (**HZDR**) [M36]
- D4.6 New hybrid models to describe the effect of solute segregation and kinetics in RPV embrittlement and aging process (**UPC) [M40]**
- D4.7 Microstructural evolution and flux effect in neutron irradiated RPV steels (**CHALM**,][M46]

Integrated Computational Materials Engineering (ICME) of RPV workflow for RPV steel and an assessment of LTO (VTT)



Ongoing: Producing computational microstructures with input data

Future: Establishing links between microstructural features and mechanical response

Ongoing: Planning of experiments with SEM in-situ tensile device; test device availability is challenging

Future: First trials with material provided by (UBRI); devicing on RPV (VTT)

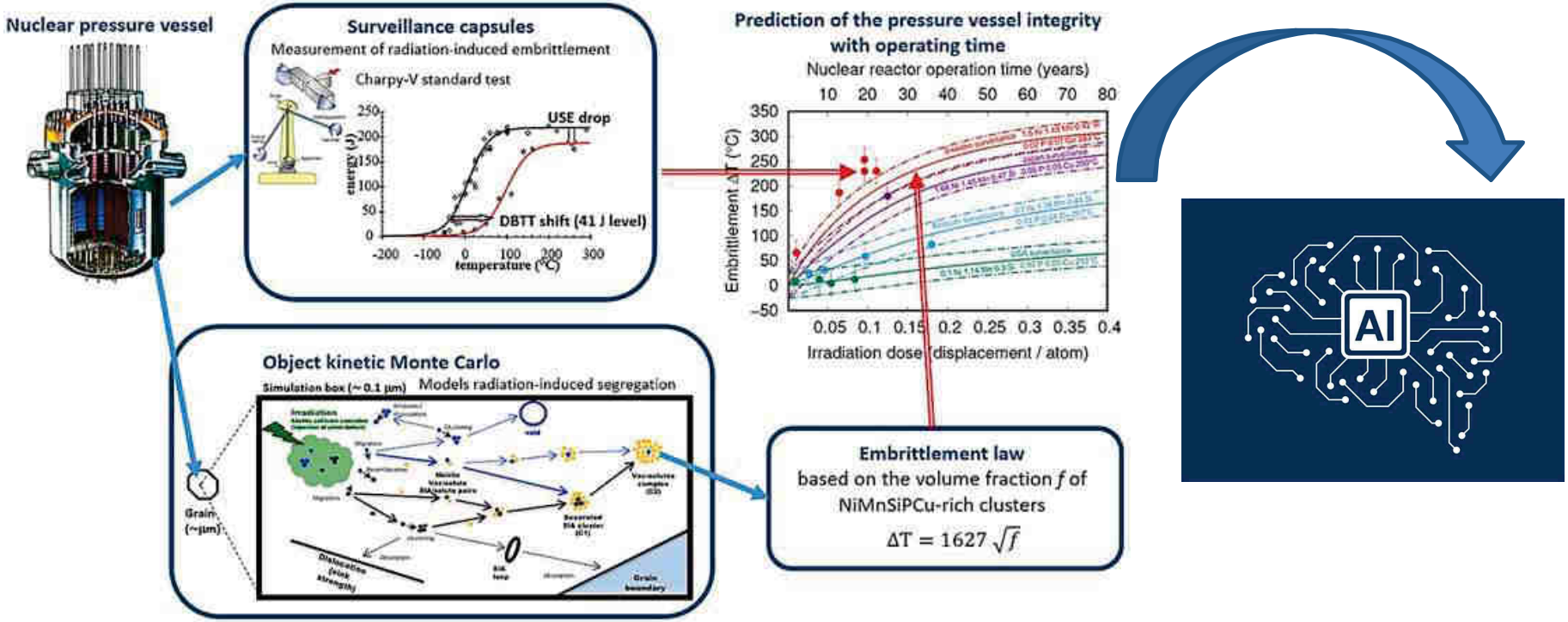
Ongoing: CP model development and tests

Future: Modifying Soteria CP framework for gradient plasticity and damage

- Inputs from WP4 ICME
- Inputs from WP3 activities
- RVE inputs from WP2

WP4 (VTT) - Accelerated model and analysis approaches

Multiscale modelling in nuclear ferritic steels: From nano-sized defects to embrittlement, N. Castin et al



101 APT measurements of *f*, *N* & *D*, from **55** irradiated steels:

- 46 P/BWR
- 6 VVER
- 3 model alloys

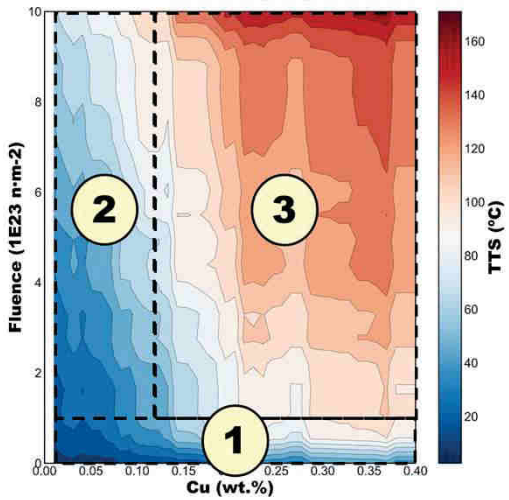
1707 experimental data from **359** irradiated steels

- 347 "Western"
- 10 VVER
- 2 model alloys

https://doi.org/10.1016/j.mtphys.2022.100802

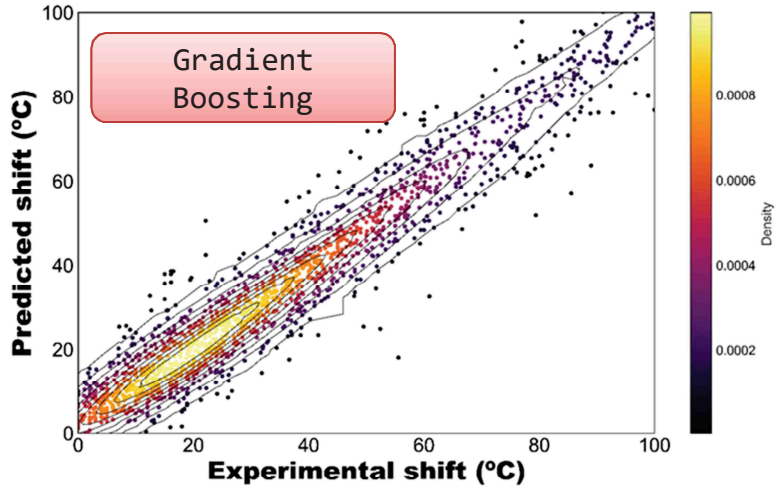
Prediction of the Transition-Temperature Shift Using Machine Learning Algorithms and the Plotter Database. D.Ferreño et al

PLOTTER ASTM Database

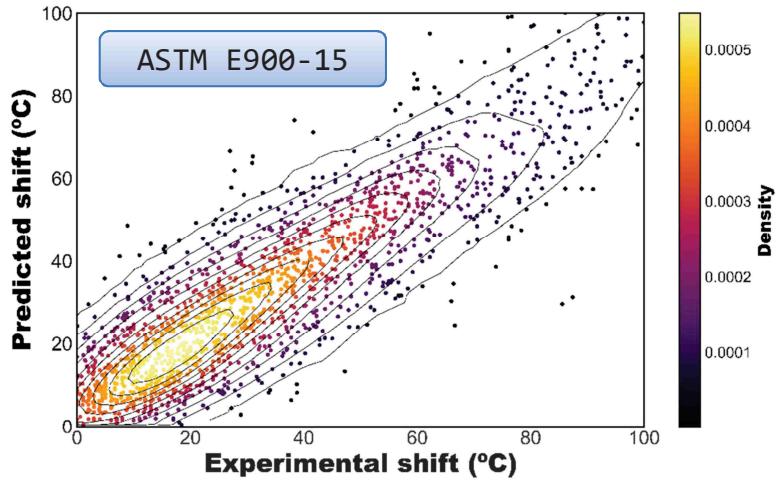


Descriptive analysis

1. For fluence < 1E+23 n·m^{-2}, embrittlement is dominated by fluence, regardless of the Cu content.
2. For fluence > 1E+23 n·m^{-2}, and Cu < 0.12%, there is an intercation between them with higuer influence from Cu.
3. In the rest of cases, the impact of fluence seems to prevail on the TTS.



(a)



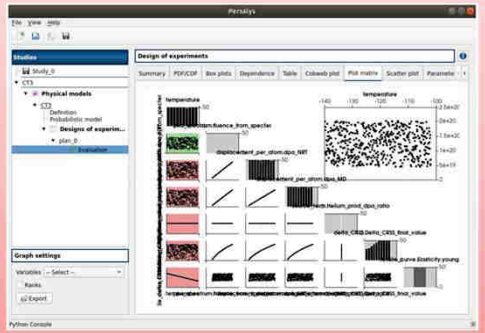
(b)

https://doi.org/10.3390/met12020186

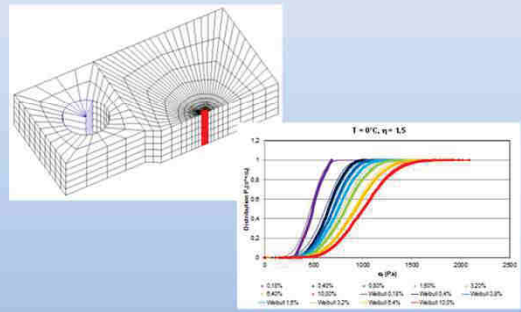
WP5 (CIEMAT) - Dissemination, exploitation and training

- **Exploitation**
  - EU and non-EU industrial partners and Technical Support Organizations (TSOs) to regulator
  - Reference cases that will include surveillance and R&D data relevant for LTO operation and Gen III/III+ RPV

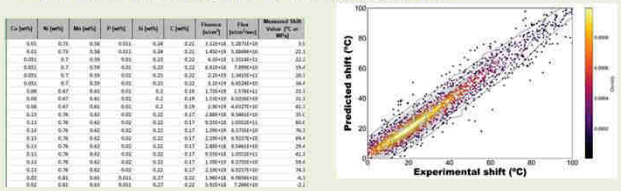
Parametric studies [SOTERIA Platform]



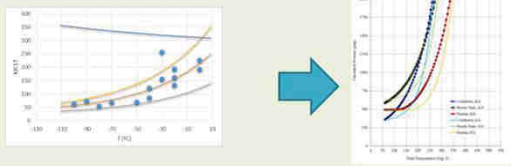
Toughness prediction : local approach to failure



Embrittlement trend curve



ASME XI Code Case N-830



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ENTENTE Exploitation Team

Horizon 2020
European Union Funding
for Research & Innovation

ENTENTE DATABASE ⟷ MatDB JRC

FORMATS

STRUMAT-LTO

Microstructure

Ni, Mn, Si ⟹ ΔT

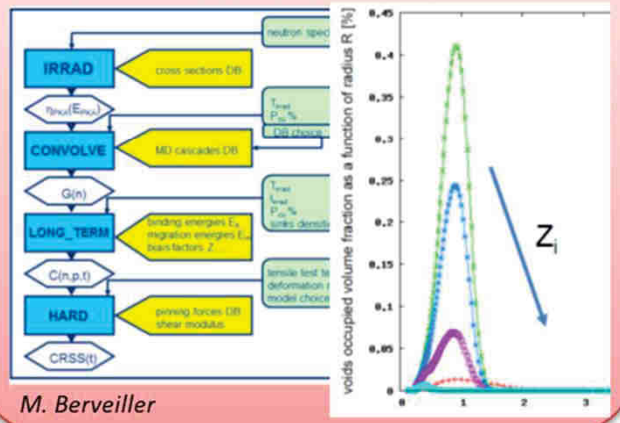
ENTENTE DATABASE

Fracture models

FRACTESUS

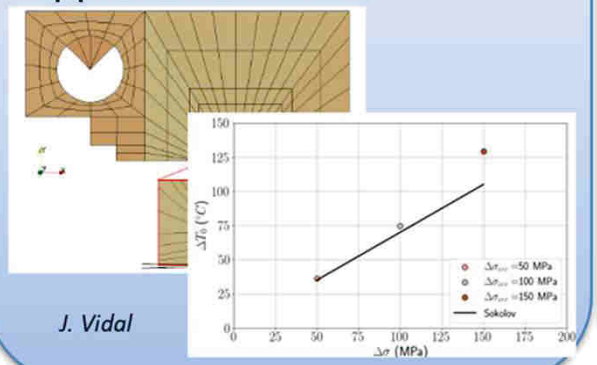
+ Machine learning methods and artificial neural networks

Microstructure evolution



M. Berveiller

Toughness prediction : local approach to failure



J. Vidal

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ENTENTE Exploitation Team

Charpy data ***FT data***

ASTM INTERNATIONAL
Helping our world work better

STRUMAT – LTO

ASME
SETTING THE STANDARD

FORMATS

FRACTESUS

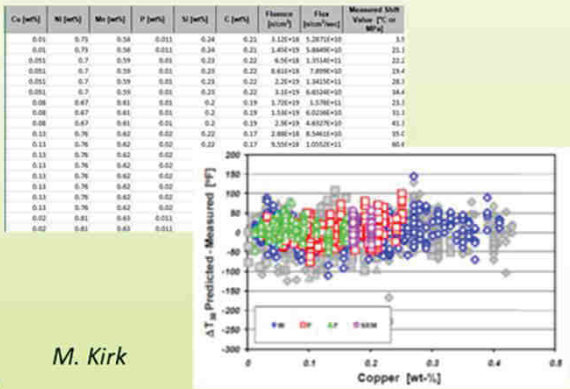
ENTENTE DATABASE

Zenodo

FT data

Horizon 2020
European Union Funding
for Research & Innovation

Embrittlement trend curve



M. Kirk

Reference cases (FRA-G)

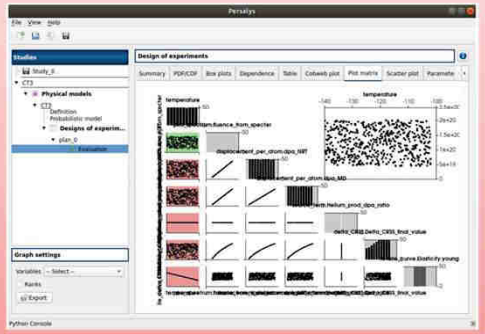
"SAMPLE PROBLEM 1, (A)" of Technical Basis report MRP-218 ⟷ -ASME Code Case N-830 Revision 1: "Case N-830-1 Direct Use of Fracture Toughness for Flaw Evaluations of Pressure Boundary Materials in Class 1 Ferritic Steel Components Section XI, Division 1".

Technical Basis report MRP-462 ⟷ -ASME Code Case N-914: ""Accounting for the Effect of Embrittlement on Fracture Toughness Properties Used in Evaluations of Pressure Boundary Materials in Class 1 Ferritic Steel Components".

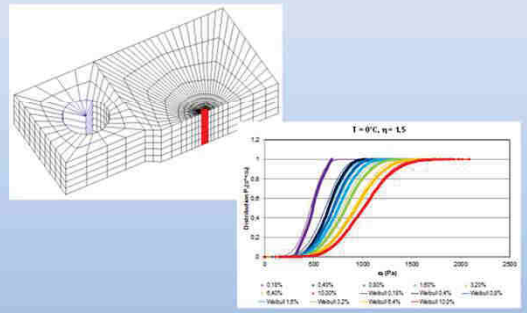
$$RT_{IRRAD} = RT_{INPUT} + Shift + M \times Margin + Offset$$

Reference case participants will be asked to calculate RT_{IRRAD} using the ENTENTE database, to provide the individual values of RT_{INPUT}, Shift, Margin, and Offset on which RT_{IRRAD} is based

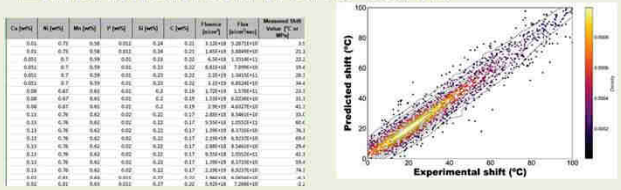
Parametric studies [SOTERIA Platform]



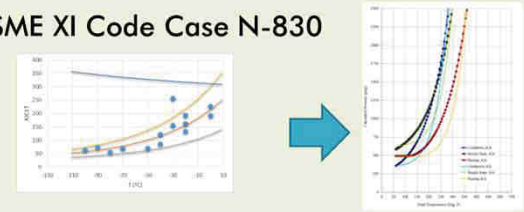
Toughness prediction : local approach to failure



Embrittlement trend curve



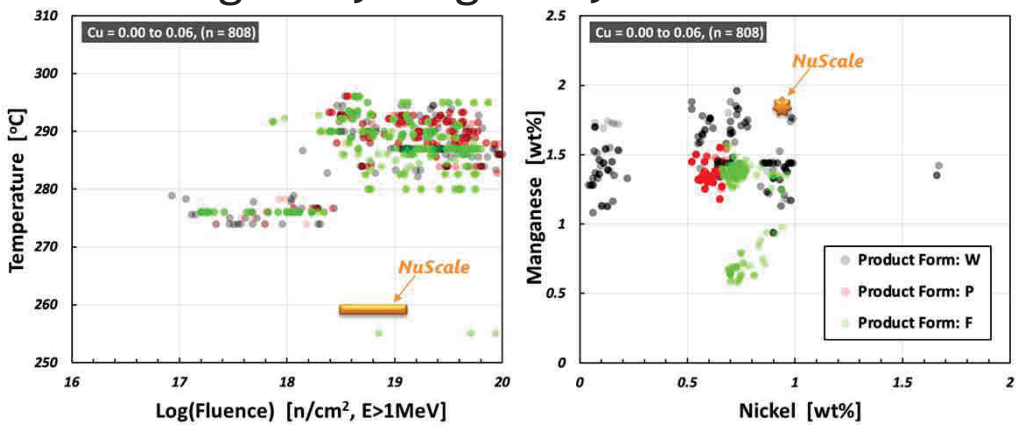
ASME XI Code Case N-830



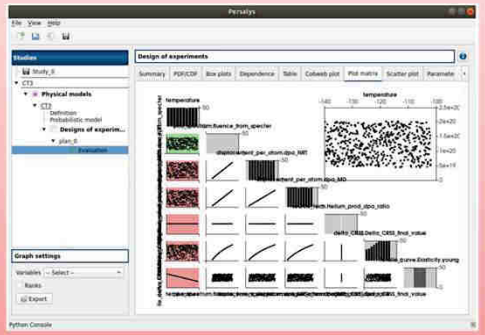
Reference cases (Mark Kirk)

- HZDR Data on Rheinsberg reactor (255ºC)
- ATUCHA Surveillance (265ºC)
- Hybrid models

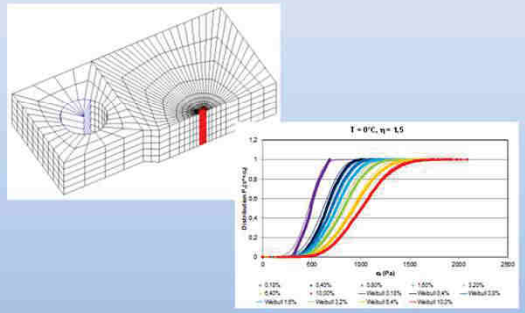
High Mn, High Ni, Low Irradiation T



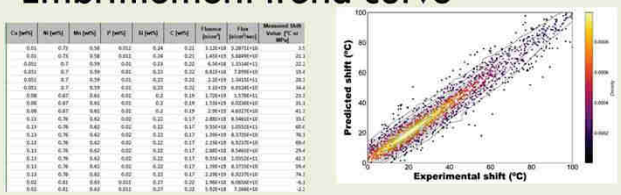
Parametric studies [SOTERIA Platform]



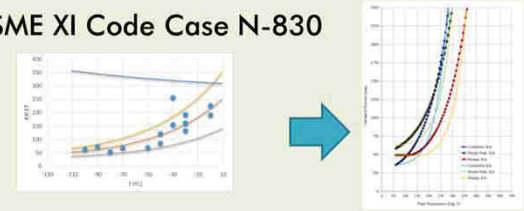
Toughness prediction : local approach to failure



Embrittlement trend curve



ASME XI Code Case N-830



SUMMARY

- ENTENTE start on 1st September 2020
- Specification of ENTENTE database is available
- The database is being populated along the project execution
- First experimental results available
- First analysis with machine learning available (published or pre-print)

This project has received funding from the Euratom research and training programme 2019-2020 under grant agreement No 900018 (ENTENTE project).