EERA
European Energy Research Alliance
Digitalisation for Energy

EERA map of data repositories, digital (AI) methodologies and numerical codes

Transversal Joint Programme
Digitalisation for Energy

January 2022

EERA map of data repositories, digital (AI) methodologies and numerical codes

Summary

This document describes a summary of the non-complete list of data repositories (22), digital (Artificial Intelligence) methodologies (24), and numerical codes (65) that are being exploited within EERA. The collection of the information described in this document comes from a brief questionnaire that for those three topics was open within the Alliance along spring 2021.

Nevertheless, this document aims at being a live one that will integrate more results and insights as new inputs are provided by the EERA researchers.

The current work has been carried out by the transversal Joint Programme Digitalisation for Energy (DfE) with the support of the EERA General Secretariat and the rest of the Joint Programmes for the dissemination of the aforementioned online questionnaire. In this sense, EERA DfE deeply acknowledges Dr. A. Bailador (CIEMAT) for implementing the online questionnaire; also, to the CIEMAT ICT Division for hosting the services and servers where the questionnaire was made available.

As mentioned before, the aim of compiling this map is counting on more complete information of what digital techniques are being exploited within EERA and, from that point on, create the basis of potential collaborations between partners which are interested in making research by means of solutions that might have been developed by others. In this sense, it is expected to avoid double efforts, create synergies, and merge and integrate common interests and developments that could derive in common lines of research.

The detailed answers provided by the different EERA groups to the questionnaire ("the map") are hosted by the EERA General Secretariat and also uploaded in the DfE documents repository at https://www.eera-set.eu/component/projects/projects.html?id=183 . There, more accurate search of results can be carried out.

The results of this questionnaire are presented in a two-fold basis. Firstly, a brief summary of repositories, methodologies, and codes are listed per category alphabetically. Secondly, the same information is both depicted and listed per EERA similar JPs, facilitating in this way synergies and potential collaborations.

List of digital tools per category

Data Repositories

Up to 22 data repositories have been reported. In what follows, the name of the repository and a brief description as provided by the person who filled the information of the questionnaire is listed. In the map, this additional information is also provided:

- The name of the person who filled the survey
- His/her e-mail address for potential contacts
- The name of the repository
- If it Is open access
- If the questionnaire is filled as either user or data provider to this repository
- The link where the repository is available
- For what purpose the repository is being used
- If the exploitation of the repository is made under any EERA JP(s) and, if so, which
- If the repository follows FAIR principles
- If the repository counts on defined metadata standards and, if so, which
- If there are any special dependencies for accessing the data or specific requirements to be used

From those answers, it is seen that:

- all of the repositories but one are open access
- 12 people are data providers actually
- 4 repositories are associated to the EERA Geothermal JP, 2 to NM, and 1 to DfE
- 14 repositories follow FAIR principles (there are 3 empty answers that could be potentially added to the previous number)
- 9 repositories counts on metadata standards
- No special dependencies are requested, but occasional embargos times and open licenses

The whole list of repositories, the institution providing the information between brackets, and a brief description follows.

1. 4TU.ResearchData (TU DELFT)
   To publish/archive research data underlying scientific publications
2. Deep Geothermal community (CNR)
   To collect and retrieve deliverables and products from EU geothermal funded project
3. e-cienciaDatos (CIEMAT)
   To deposit the data of a scientific article

4. ERA5 (CIEMAT)
   Source for meteorological data
5. Geothermcatalog (CNR)
   To catalogue Italian Geothermal datasets
6. GFZ Data Services (GFZ POSTDAM)
   Data archiving and publication, valid for assessing already published data.
7. Global Heat Flow Database (GFZ POSTDAM)
   Compiling the IHFC compilation of the global heat flow data
8. IEA PVPS Task 13 Data Base (AIT)
   Performance, Operation and Reliability of Photovoltaic Systems
9. INESC TEC research data repository (INESC TEC)
   Open data policy at INESC TEC
10. International Criticality Safety Benchmark Evaluation Project – ICSBEP (CIEMAT)
    Nuclear energy oriented research
11. JANIS (CIEMAT)
    Visualizing nuclear data for nuclear energy oriented research
12. Materials project (UNIOVI)
    Check on known systems to aid in computational materials design
13. ODIN Portal (EUROPEAN COMMISSION)
    Managing engineering materials test data coming from EU research and industry.
14. PED Labs UE (CIEMAT)
    COST ACTION PED UE NET
15. PetroPhysical Property Database P3 (TU DARMSTADT)
    Reservoir rock characterization
16. PVGIS (AIT - CIEMAT)
    This data bank delivers PV performance and solar radiation data in the areas covered by Meteosat and GOES satellite and also provides tools running on this DB.
17. Repositório LNEG (LNEG)
    Obtain references and read articles
18. RISIS (AIT)
    Analyses for research & innovation policy
19. ViMiLabs (FZJ)
    Materials discovery
20. Energy data platforms (HVL and EERAdata project)
    Compilation of databases related to buildings efficiency, power transmission & distribution networks, material efficiency, and energy and energy efficiency policies

Methodologies

Up to 24 digital (AI) methodologies have been reported. In what follows, the name of the methodology and a brief description as provided by the person who filled the information of the methodology is listed. In the map, this additional information is also provided:

- The name of the person who filled the survey
- His/her e-mail address for potential contacts
- The name of the methodology (for example, neural network, solver, etc.)
- If it is open source
- If the person who filled the questionnaire is one of the developers/owners of the methodology
- A link where this methodology is available, if any
- For what purpose this methodology is being used
- If the exploitation of the methodology is made under any EERA JP(s) and, if so, which
- If there are any special dependencies for running the methodology (for example, OS version, additional libraries, etc.)

From those answers, it is seen that:

- 11 methodologies are open source, being assumed that the rest can be jointly exploited by new groups under a collaboration scheme
- 11 methodologies have been developed by the proposing person
- The EERA NM JP is exploiting 2 methodologies and FCH JP is exploiting an additional one.
- Some of the requirements associated to these methodologies are the use of Matlab, VBA language, Anaconda, etc.

The whole list of methodologies, the institution providing the information between brackets, and a brief description follows.

1. Atomistic codes (UNIOVI)
   Tools and Python modules for setting up, manipulating, running, visualizing, and analysing atomistic simulations
2. Calphad (UNITO)
   Assessment of thermodynamic properties and phase diagram
3. CAnELA (CIEMAT)
   Analysis of spectral lines for measuring intensity, widths, Gaussian and Lorentzian components, etc.
4. Drilling automatization (FRAUNHOFFER)
5. EOF, CCA and cluster analysis (CIEMAT)
   Studies of variability, uncertainty, regionalization...
6. Energy Storage Systems: Dimensioning methodology– ESS (CIEMAT)
   The ESS dimensioning methodology is based on a mathematical optimization problem solver based on a Differential Evolutionary Algorithm. This solver has

been tested with different problems: - Dimensioning the energy storage capacity of an autonomous wave energy converter - Dimensioning the energy storage capacity of a wave energy farm in order to comply with grid codes. - Dimensioning the energy storage capacity for an industrial installation in order to optimise the economic investment.

7. Energy time series forecasting toolbox (INESTEC)
   R&D projects and software development for forecasting companies (technology transfer)
8. European Geothermal Research and Innovation Search Engine – EGRISE (CNR)
   To retrieve products from EU geothermal funded projects
9. Framework for Integrated Sustainability Assessment – FISA (CIEMAT)
   Assessing sustainability indicators of energy investments
10. Gamma spectrometry: Solver to adjust peaks in (CIEMAT)
    Applications of VBA_excel (Visual Basic for applications) for calculating activity concentration and to validate results for accreditation. Effort to connect the computers to scales, alpha spectrometer and validation techniques. Methodology to add spectrum and to improve sensitivity of methods and detection of radionuclides in air.
11. Geothermal resource assessment by Favourability maps (CNR)
    To predict the best location to install a geothermal power plant, including data integration for geothermal resource assessment and cluster analysis of geophysical datasets
12. Materials characterization (POLITO)
    Materials characterization
13. Materials science (UNIOVI)
    Multipurpose tool for computational nuclear materials simulations
14. Method and device for preserving privacy of linear regression distributed learning (INESTEC)
15. Smart4RES EU project and software development for different use cases like forecasting and voltage control
16. Modelica: First principles object-oriented modelling and simulation (CIEMAT)
    Dynamic modelling of solar thermal power plants, for: analysis, advanced control design, optimization, and any other application of the models developed (for example: artificial intelligence).
17. Multiscale modelling of electrochemical data (DIFFER)
    Multiscale modelling of electrochemical data
18. Navier Stokes solver (CIEMAT)
    Simulation of flames and reacting flows, simulation of heat transfer
19. Neural networks (convolutional, deep, recurrent...) for load disaggregation (TU CLAUSTHAL)
    Smart meter data analytics
20. Planning (LNEG)
    Offshore planning

21. Reduced Graphene Oxide Synthesis (CIEMAT)
    The methodology provides graphene materials for different projects related the development of sulphur gas adsorbents, solar cells, hydrogen storage and supercapacitors.
22. Stata econometrics (UCD)
23. Tensorflow (VTT)
    Flaw detection in ultrasonic data

Numerical codes

Up to 65 numerical codes have been reported (additional incomplete information has been also provided, but it is not integrated in this summary). In what follows, the name of the codes and a brief description as provided by the person who filled the information of the code is listed. In the map, this additional information is also provided:

- The name of the person who filled the survey
- His/her e-mail address for potential contacts
- The name of the code
- If it is open source
- If the person who filled the questionnaire is one of the developers/owners of the code
- A link where this code is available, if any
- For what purpose this code is being used
- If the exploitation of the code is made under any EERA JP(s) and, if so, which
- If there are any special dependencies for running the code (for example, OS version, additional libraries, etc.)

From those answers, it is seen that:

- 24 codes are open source, being assumed that the rest can be jointly exploited
- 27 codes have been developed by the proposing person
- 10 Codes are being exploited under the EERA AMPEA (2), ESI (2), Geothermal (2), E3S (1), NM (3), Smart Grids (1), and Wind (1) JPs
- Most of the codes are run in Linux-based environment.

The whole list of codes, the institution providing the information between brackets, and a brief description follows.

1. ABAQUS (EUROPEAN COMMISSSION)
   Structural mechanics modelling: static, dynamic stress analyses, fatigue and creep-fatigue analyses, fracture mechanics, development of advanced constitutive models (crystal plasticity, strain gradient crystal plasticity), multi-scale modelling.

2. ABINIT (CEA)
   Electronic structure calculations on nuclear fuels

3. Alya (BSC-CNS)
   Wind resource assessment.

4. ANSYS-CFX / ANSYS-FLUENT / ANSYS-ICEMCFD / ZView (U. SEVILLA - CIEMAT)
   ANSYS-CFX: Computational Fluid Dynamics modelling and simulation
   For performing CFD calculations mainly focussed on MHD and buoyancy interaction in PbLi flows inside fusion breeding blankets

5. ASCOT (CIEMAT)
   Simulations of fast-ion confinement in magnetically confined fusion devices

6. ASTEC (CIEMAT)
   Numerical simulations for severe accident phenomena in nuclear power plants

7. CRESCENDO (CEA)
   Cluster dynamics simulation of diffusion in nuclear fuels

8. CRYSTAL14 (CSIC - UNITO)
   Computing interfaces between photocatalytic solids. Quantum mechanical modelling of periodic systems (solids, surfaces, polymers, nanotubes, nanoparticles, clusters) with many applications in materials science. In details, the CRYSTAL program computes the electronic structure of periodic systems within Hartree Fock, density functional or various hybrid approximations (global, range-separated and double-hybrids). The Bloch functions of the periodic systems are expanded as linear combinations of atom centred Gaussian functions. Powerful screening techniques are used to exploit real space locality.

9. DYMOKA (U. LILLE)
   MD simulations

10. Ecosim (CIEMAT)
    Tritium breeding blanket modelling and simulations

11. EnergyBox (IREC)
    Energy management system for microgrids including ESS, V2G, RES, and different load types.

12. Energysim (TU DELFT)
    energysim is a Python package which runs continuous time simulation of energy systems (electricity, heat, gas, etc.) using FMU wrapped models. The environment is particularly suitable for exploring flexibility of multi-energy systems, from quantification of this flexibility to its engagement through various control and coordination actions.

13. Energy Storage Systems (ESS) Loss Model Set (CIEMAT)
    Supercapacitors, flywheel, batteries… A Model to be used in control development, optimization process, or grid integration analysis (in-house codes are developed based on e.g. MATLAB and / or SIMULINK).

14. EUTERPE (CIEMAT)
    Gyrokinetic simulations of plasma turbulence in stellarators

15. EVOLCODE (CIEMAT)
    Calculation of isotopic evolution of nuclear reactors

16. FHI-AIMS (CSIC)
    To compute energies of solids and molecules

17. FRAPCON (CIEMAT)
    For research on fuel thermo-mechanical performance

18. FRAPTRAN (CIEMAT)
    For research on fuel thermo-mechanical performance under transient conditions

19. Gempy (RWTH-AACHEN)
    GemPy is a Python-based, open-source geomodelling library. It is capable of constructing complex 3D geological models of folded structures, fault networks and unconformities, based on the underlying powerful implicit representation approach. We use it to obtain representations of relevant subsurface structures for geothermal energy use.

20. GOLEM a MOOSE-base application (GFZ-POSTDAM)
    Highly scalable (MPI) Thermal-Hydraulic-Mechanical and non-reactive chemistry plus rate and state frictional fault behaviour modelling of fractured reservoirs.

21. GridapMHD (CIEMAT)
    MHD computations of liquid metal flows under strong magnetic fields assuming inductionless approximation

22. HOMER Pro (CIEMAT)
    Analysis and design of renewable energy systems

23. KINECLUE (CEA)
    Modelling of diffusion and transport properties of nuclear materials and especially nuclear fuels

24. KNOSOS (CIEMAT)
    Numerical calculation of transport in fusion plasmas.

25. LAMMPS (CEA, UPC, UNIOVI)
    Atomic scale modelling of properties and behaviour of nuclear fuels. Also, to perform MD simulations of materials interesting for nuclear applications.

26. Libradtran (CIEMAT)
    It is a radiative transfer code, it solves the radiative transfer equation in atmospheric layers; it also can solve the LIDAR equation.

27. MCNP (CIEMAT)
    Particle transport calculations for nuclear energy oriented research. Nuclear transport calculations for the nuclear (Fusion or Fission) design facilities

28. MELCOR (CIEMAT)
    Numerical simulation for severe accident in nuclear power plants. Thermal-hydraulic simulations applied to accident analysis within the IFMIF-DONES project.

29. MOLDRAW (UNITO)
    A program to display and manipulate molecular and crystalline structures.
    This program allows visualizing and manipulating the structure of molecules and crystals. Furthermore, it can prepare input and read output from many quantum mechanical programs (MOPAC, Gaussian, CRYSTAL, VASP, xTB)

30. Multiscale modelling of electrochemical data (DIFFER)
    Multiscale modelling of electrochemical data

31. MUST-AeroVIEW (CENER)
    Integrated analysis of floating wind turbines with several rotors. The tool allows considering the rotor-wake interaction and also the interaction between wakes of nearby rotors.

32. NJOY (CIEMAT)
    Nuclear data processing for nuclear-energy oriented research

33. NUMODIS (CEA)
    Dislocation Dynamics code dedicated to the simulation of plasticity at the grain level in a wide range of materials including BCC, FCC and HCP crystallographic structures.

34. OPenFOAM (CIEMAT)
    3 dimensional simulations of combustion problems.

35. OpenFoam (CENER)

Wind turbine aerodynamic computations, and wind turbine platform hydrodynamic computations

36. Optica (CIEMAT)
    Fitting Reflectance, back Reflectance, and, or Transmittance of a multilayer to a physical model.

37. PENELOPE (CIEMAT)
    Simulation ionizing radiation detector

38. Phonons Monte Carlo (U. LORRAINE)
    Computing thermal transport properties of semiconductors

39. PLATOON (CIEMAT)
    Thermal-hydraulic modelling at system level in fusion breeding blankets

40. PorePy (UIB)
    Simulation of coupled thermo-hydro-mechanical-chemical processes in fractured porous media, including fracture deformation and propagation.

41. PSSTool (LEI)
    The Prosumer Solution Simulation tool performs a technical and economic analysis about integrating photovoltaic (PV) systems into households, offices, industries and other type of buildings. Every case is addressed differently, since energy consumption and the demand profile varies from case to case. Moreover, hourly discrimination tariffs and the technical aspects these PV systems must comply with usually depend on the size of the system.

42. Q2DHS (CIEMAT)
    Flame dynamics calculation in a Hele-Shaw cell configuration

43. Quantum Espresso 6.6 (CSIC)
    Computing U values for DFT+U approaches, g tensor values obtained in EPR experiments using the gipaw approach, and GW methods using the West code; and, in general, for other purposes of solid calculations

44. SCALE (CIEMAT)
    Nuclear energy-oriented research.

45. SERPENT (CIEMAT)
    Particle transport calculations for nuclear energy oriented research.

46. SHEMAT-Suite (RWTH-AACHEN)

SHEMAT-Suite (Simulator for HEat and MAss Transport) is a code for computing flow, heat and species transport equations in porous media. The governing equations of the code are the groundwater flow equation, the heat transport equation and the species transport equation.

47. Smart Software Tool for Electricity Mix Optimization (SMARTMIX) (CIEMAT-PSA)
    A software tool based on historical data and artificial intelligence (genetic algorithms) to optimize the electricity mix. It performs a multiobjective optimization, minimizing simultaneously the electricity cost and curtailments, while matching the required hourly demand and keeping the CO2 emissions in a desired range.

48. Stella (CIEMAT)
    For research purposes. Study of turbulence in thermonuclear fusion plasmas.

49. STELLOPT (CIEMAT)
    Optimization of stellarator configurations

50. TIMES (CIEMAT)
    Energy systems optimization

51. tkwantoperator (CEA)
    To simulate energy/heat transport carried by electrons in time-dependent quantum systems

52. TR_EVOL (CIEMAT)
    Estimation of mass balance and cost of nuclear fuel cycle scenarios. Modelling and study of electronuclear scenarios

53. VASP 6.x (CEA, CSIC, UNIOVI)
    Electronic structure calculations on nuclear fuels and structural nuclear materials. Also, computing structures and energies of different solids (CuOx/CeO2, interfaces between semiconductors and photocatalysts (Ce,Zr)O2, etc.)

54. VITALITY Plugin, within Grasshopper / Rhino environment (AIT)
    Tool for optimized placing of PV panels within the building envelope, considering (local) solar resource and self-consumption

List of digital tools per EERA JP

The same information is also grouped per JPs in order to facilitate synergies and awareness of the different developments that are being exploited within the Alliance.

In what follows, the digital artefacts (repositories, methodologies, and/or codes) are listed in this way, but a couple of graphical representations are depicted first.

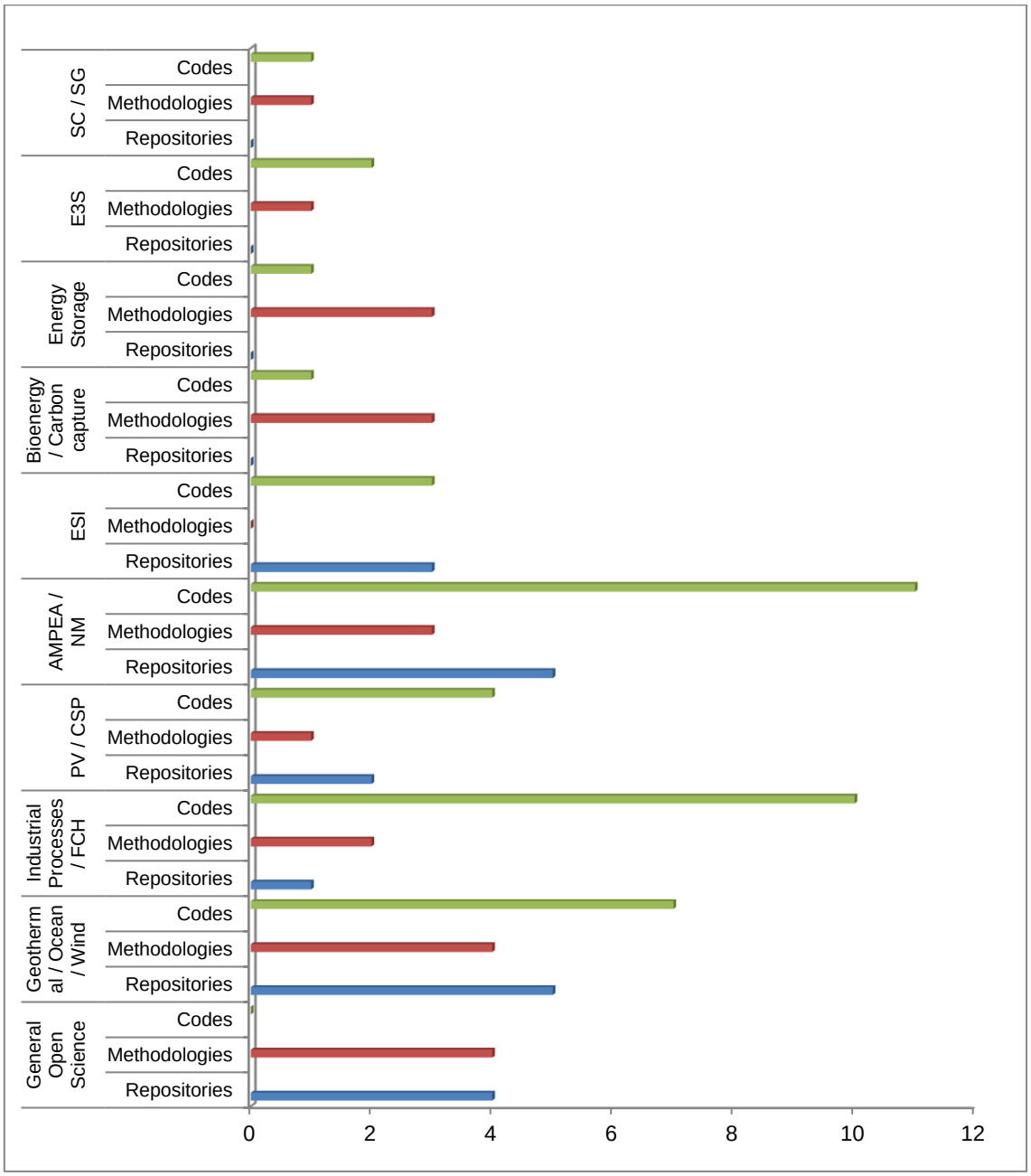

Fig 1. Number of entries per digital artefact and associated JP

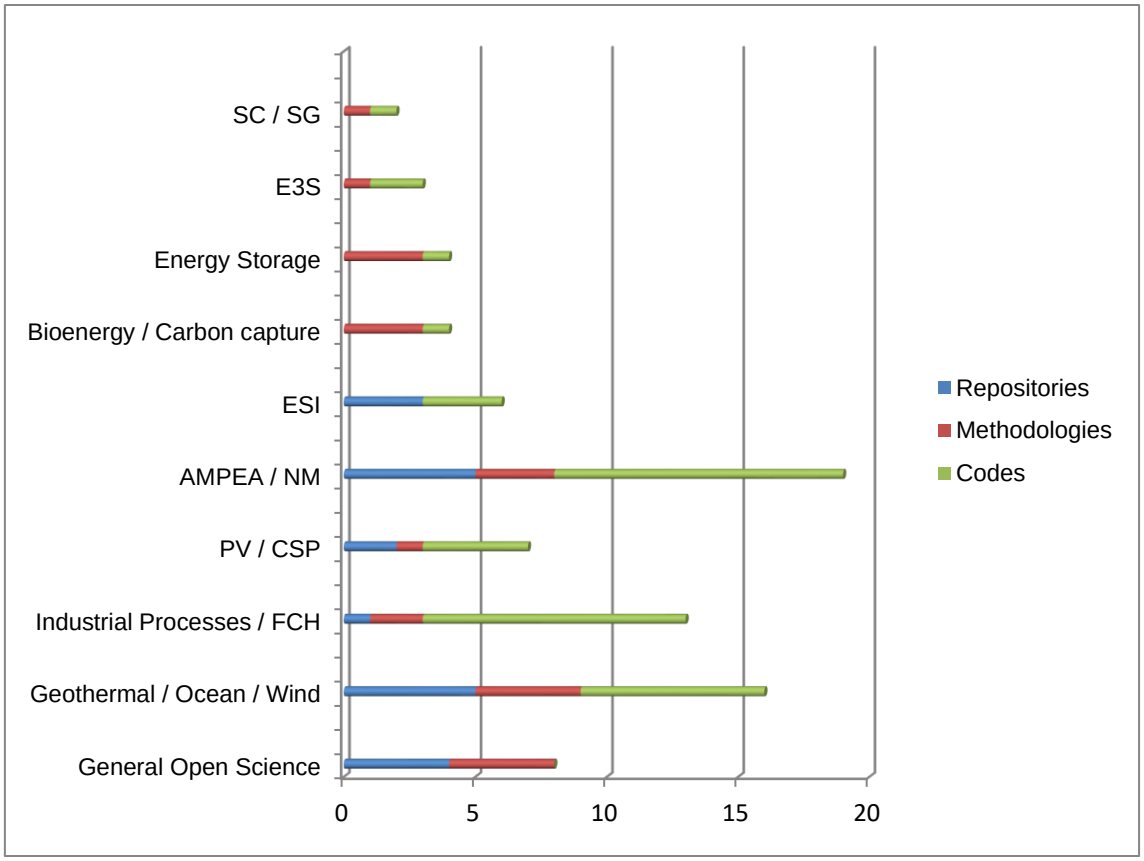

Fig 2. Number of entries per digital artefact and associated JP (cumulative)

General Open Science

Repositories

4TU.ResearchData (TU DELFT)
To publish/archive research data underlying scientific publications
e-cienciaDatos (CIEMAT)
To deposit the data of a scientific article
INESC TEC research data repository (INESC TEC)
Open data policy at INESC TEC
Repositório LNEG (LNEG)
Obtain references and read articles

Methodologies

EOF, CCA and cluster analysis (CIEMAT)
Studies of variability, uncertainty, regionalization...
Energy time series forecasting toolbox (INESTEC)
R&D projects and software development for forecasting companies (technology transfer)
Method and device for preserving privacy of linear regression distributed learning (INESTEC)
Smart4RES EU project and software development for different use cases like forecasting and voltage control
Tensorflow (VTT)
Flaw detection in ultrasonic data

Geothermal / Ocean / Wind

Repositories

Deep Geothermal community (CNR)
: To collect and retrieve deliverables and products from EU geothermal funded project

ERA5 (CIEMAT)
: Source for meteorological data

Geothermcatalog (CNR)
: To catalogue Italian Geothermal datasets

GFZ Data Services (GFZ POSTDAM)
: Data archiving and publication, valid for assessing already published data.

PetroPhysical Property Database P3 (TU DARMSTADT)
: Reservoir rock characterization

Methodologies

Drilling automatization (FRAUNHOFFER)
: Drilling processes

European Geothermal Research and Innovation Search Engine – EGRISE (CNR)
: To retrieve products from EU geothermal funded projects

Geothermal resource assessment by Favourability maps (CNR)
: To predict the best location to install a geothermal power plant, including data integration for geothermal resource assessment and cluster analysis of geophysical datasets

Planning (LNEG)
: Offshore planning

Codes

Alya (BSC-CNS)
: Wind resource assessment.

Gempy (RWTH-AACHEN)
: GemPy is a Python-based, open-source geomodelling library. It is capable of constructing complex 3D geological models of folded structures, fault networks and unconformities, based on the underlying powerful implicit representation approach. We use it to obtain representations of relevant subsurface structures for geothermal energy use.

GOLEM a MOOSE-base application (GFZ-POSTDAM)
: Highly scalable (MPI) Thermal-Hydraulic-Mechanical and non-reactive chemistry plus rate and state frictional fault behaviour modelling of fractured reservoirs.

Libradtran (CIEMAT)
: It is a radiative transfer code, it solves the radiative transfer equation in atmospheric layers; it also can solve the LIDAR equation.

MUST-AeroVIEW (CENER)
: Integrated analysis of floating wind turbines with several rotors. The tool allows considering the rotor-wake interaction and also the interaction between wakes of nearby rotors.

OpenFoam (CENER)
: Wind turbine aerodynamic computations, and wind turbine platform hydrodynamic

PorePy (UIB)
: Simulation of coupled thermo-hydro-mechanical-chemical processes in fractured porous media, including fracture deformation and propagation.

Industrial Processes / Fuel Cells and Hydrogen

Repositories

Global Heat Flow Database (GFZ POSTDAM)
Compiling the IHFC compilation of the global heat flow data

Methodologies

Calphad (UNITO)
Assessment of thermodynamic properties and phase diagram
Navier Stokes solver (CIEMAT)
Simulation of flames and reacting flows, simulation of heat transfer

Codes

ANSYS-CFX / ANSYS-FLUENT / ANSYS-ICEMCFD / ZView (U. SEVILLA - CIEMAT)
ANSYS-CFX: Computational Fluid Dynamics modelling and simulation for performing CFD calculations mainly focussed on MHD and buoyancy interaction in PbLi flows inside fusion breeding blankets
FHI-AIMS (CSIC)
To compute energies of solids and molecules
FRAPCON (CIEMAT)
For research on fuel thermo-mechanical performance
FRAPTRAN (CIEMAT)
For research on fuel thermo-mechanical performance under transient conditions
NUMODIS (CEA)
Dislocation Dynamics code dedicated to the simulation of plasticity at the grain level in a wide range of materials including BCC, FCC and HCP crystallographic structures.
OPenFOAM (CIEMAT)
3 dimensional simulations of combustion problems.
Q2DHS (CIEMAT)
Flame dynamics calculation in a Hele-Shaw cell configuration
SHEMAT-Suite (RWTH-AACHEN)
SHEMAT-Suite (Simulator for HEat and MAss Transport) is a code for computing flow, heat and species transport equations in porous media. The governing equations of the code are the groundwater flow equation, the heat transport equation and the species transport equation.
tkwantoperator (CEA)
To simulate energy/heat transport carried by electrons in time-dependent quantum systems
VASP 6.x (UNIOVI)
Computing structures and energies of different solids (CuOx/CeO2, interfaces between semiconductors and photocatalysts (Ce,Zr)O2, etc.)

Photovoltaics / Concentrated Solar Power

Repositories

IEA PVPS Task 13 Data Base (AIT)
Performance, Operation and Reliability of Photovoltaic Systems
PVGIS (AIT - CIEMAT)

This data bank delivers PV performance and solar radiation data in the areas covered by Meteosat and GOES satellite and also provides tools running on this DB.

Methodologies

Modelica: First principles object oriented modelling and simulation (CIEMAT)

Dynamic modelling of solar thermal power plants, for: analysis, advanced control design, optimization, and any other application of the models developed (for example: artificial intelligence).

Codes

CRYSTAL14 (CSIC - UNITO)

Computing interfaces between photocatalytic solids. Quantum mechanical modelling of periodic systems (solids, surfaces, polymers, nanotubes, nanoparticles, clusters) with many applications in materials science. In details, the CRYSTAL program computes the electronic structure of periodic systems within Hartree Fock, density functional or various hybrid approximations (global, range-separated and double-hybrids). The Bloch functions of the periodic systems are expanded as linear combinations of atom centred Gaussian functions. Powerful screening techniques are used to exploit real space locality.

MOLDRAW (UNITO)

A program to display and manipulate molecular and crystalline structures. This program allows visualizing and manipulating the structure of molecules and crystals. Furthermore, it can prepare input and read output from many quantum mechanical programs (MOPAC, Gaussian, CRYSTAL, VASP, xTB)

Optica (CIEMAT)

Fitting Reflectance, back Reflectance, and, or Transmittance of a multilayer to a physical model.

VITALITY Plugin, within Grasshopper / Rhino environment (AIT)

Tool for optimized placing of PV panels within the building envelope, considering (local) solar resource and self-consumption

AMPEA / Nuclear Materials

Repositories

International Criticality Safety Benchmark Evaluation Project – ICSBEP (CIEMAT)

Nuclear energy oriented research

JANIS (CIEMAT)

Visualizing nuclear data for nuclear energy oriented research

Materials project (UNIOVI)

Check on known systems to aid in computational materials design

ODIN Portal (EUROPEAN COMMISSION)

Managing engineering materials test data coming from EU research and industry.

ViMiLabs (FZJ)

Materials discovery

Methodologies

Atomistic codes (UNIOVI)

Tools and Python modules for setting up, manipulating, running, visualizing, and analysing atomistic simulations

Materials characterization (POLITO)

Materials characterization

Materials science (UNIOVI)

Multipurpose tool for computational nuclear materials simulations

Codes

ABAQUS (EUROPEAN COMMISSSION)

Structural mechanics modelling: static, dynamic stress analyses, fatigue and creep-fatigue analyses, fracture mechanics, development of advanced constitutive models (crystal plasticity, strain gradient crystal plasticity), multi-scale modelling.

ABINIT (CEA)

Electronic structure calculations on nuclear fuels

ASTEC (CIEMAT)

Numerical simulations for severe accident phenomena in nuclear power plants

CRESCENDO (CEA)

Cluster dynamics simulation of diffusion in nuclear fuels

DYMOKA (U. LILLE)

MD simulations

KINECLUE (CEA)

Modelling of diffusion and transport properties of nuclear materials and especially nuclear fuels

LAMMPS (CEA, UPC, UNIOVI)

Atomic scale modelling of properties and behaviour of nuclear fuels. Also, to perform MD simulations of materials interesting for nuclear applications.

NJOY (CIEMAT)

Nuclear data processing for nuclear-energy oriented research

Phonons Monte Carlo (U. LORRAINE)

Computing thermal transport properties of semiconductors

Quantum Espresso 6.6 (CSIC)

Computing U values for DFT+U approaches, g tensor values obtained in EPR experiments using the gipaw approach, and GW methods using the West code; and, in general, for other purposes of solid calculations

VASP 6.x (CEA, CSIC)

Electronic structure calculations on nuclear fuels and structural nuclear materials.

Energy Systems Integration

Repositories

PED Labs UE (CIEMAT)

COST ACTION PED UE NET

RISIS (AIT)

Analyses for research & innovation policy

Energy data platforms (HVL and EERAdata project)

Compilation of databases related to buildings efficiency, power transmission & distribution networks, material efficiency, and energy and energy efficiency policies

Codes

Energysim (TU DELFT)

energysim is a Python package which runs continuous time simulation of energy systems (electricity, heat, gas, etc.) using FMU wrapped models. The environment is particularly suitable for exploring flexibility of multi-

energy systems, from quantification of this flexibility to its engagement through various control and coordination actions.

HOMER Pro (CIEMAT)

Analysis and design of renewable energy systems

Smart Software Tool for Electricity Mix Optimization (SMARTMIX) (CIEMAT-PSA)

A software tool based on historical data and artificial intelligence (genetic algorithms) to optimize the electricity mix. It performs a multiobjective optimization, minimizing simultaneously the electricity cost and curtailments, while matching the required hourly demand and keeping the CO2 emissions in a desired range.

Bioenergy / Carbon capture and storage

Methodologies

Gamma spectrometry: Solver to adjust peaks in (CIEMAT)

Applications of VBA_excel (Visual Basic for applications) for calculating activity concentration and to validate results for accreditation.

CAnELA (CIEMAT)

Analysis of spectral lines for measuring intensity, widths, Gaussian and Lorentzian components, etc.

Multiscale modelling of electrochemical data (DIFFER)

Multiscale modelling of electrochemical data

Codes

Multiscale modelling of electrochemical data (DIFFER)

Multiscale modelling of electrochemical data

Energy storage

Methodologies

Energy Storage Systems: Dimensioning methodology– ESS (CIEMAT)

The ESS dimensioning methodology is based on a mathematical optimization problem solver based on a Differential Evolutionary Algorithm.

Stata econometrics (UCD)

Econometrics calculi

Reduced Graphene Oxide Synthesis (CIEMAT)

The methodology provides graphene materials for different projects related the development of sulphur gas adsorbents, solar cells, hydrogen storage and supercapacitors.

Codes

Energy Storage Systems (ESS) Loss Model Set (CIEMAT)

Supercapacitors, flywheel, batteries… A Model to be used in control development, optimization process, or grid integration analysis (in-house codes are developed based on e.g. MATLAB and / or SIMULINK).

E3S

Methodologies

Framework for Integrated Sustainability Assessment – FISA (CIEMAT)

Assessing sustainability indicators of energy investments

Codes

PSSTool (LEI)

The Prosumer Solution Simulation tool performs a technical and economic analysis about integrating photovoltaic (PV) systems into households, offices, industries and other type of buildings. Every case is addressed differently, since energy consumption and the demand profile varies from case to case. Moreover, hourly discrimination tariffs and the technical aspects these PV systems must comply with usually depend on the size of the system.

TIMES (CIEMAT)

Energy systems optimization

Smart Cities / Smart Grids

Methodologies

Neural networks (convolutional, deep, recurrent...) for load disaggregation (TU CLAUSTHAL)

Smart meter data analytics

Codes

EnergyBox (IREC)

Energy management system for microgrids including ESS, V2G, RES, and different load types.

(Partially) Out of the scope of EERA JPs

Codes

ASCOT (CIEMAT)

Simulations of fast-ion confinement in magnetically confined fusion devices

Ecosim (CIEMAT)

Tritium breeding blanket modelling and simulations

EUTERPE (CIEMAT)

Gyrokinetic simulations of plasma turbulence in stellarators

EVOLCODE (CIEMAT)

Calculation of isotopic evolution of nuclear reactors

GridapMHD (CIEMAT)

MHD computations of liquid metal flows under strong magnetic fields assuming inductionless approximation

KNOSOS (CIEMAT)

Numerical calculation of transport in fusion plasmas.

MCNP (CIEMAT)

Particle transport calculations for nuclear energy-oriented research. Nuclear transport calculations for the nuclear (Fusion or Fission) design facilities

MELCOR (CIEMAT)

Numerical simulation for severe accident in nuclear power plants. Thermal-hydraulic simulations applied to accident analysis within the IFMIF-DONES project.

PENELOPE (CIEMAT)

Simulation ionizing radiation detector

PLATOON (CIEMAT)

Thermal-hydraulic modelling at system level in fusion breeding blankets

SCALE (CIEMAT)

Nuclear energy-oriented research.

SERPENT (CIEMAT)

Particle transport calculations for nuclear energy oriented research.

Stella (CIEMAT)

For research purposes. Study of turbulence in thermonuclear fusion plasmas.

STELLOPT (CIEMAT)

Optimization of stellarator configurations

TR_EVOL (CIEMAT)

Estimation of mass balance and cost of nuclear fuel cycle scenarios. Modelling and study of electronuclear scenarios