



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

Transversal Joint Programme
Digitalisation for Energy

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EERA MAP OF DATA REPOSITORIES, DIGITAL (AI) METHODOLOGIES, AND NUMERICAL CODES

SUMMARY

This document describes an updated summary of the non-complete list of data repositories (26), digital (Artificial Intelligence) methodologies (35), and numerical codes (68) that are being exploited within EERA, as those of 2023. The collection of information described in this document comes from a brief questionnaire that for those three topics was open within the Alliance along May 2023. It updates and complements the one already carried out during the spring of 2021.

Hence, 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 to count on more complete information on 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 result 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 to the DfE documents repository at their specific webpage. There, a more accurate search of results can be carried out.

The results of this questionnaire are presented on a two-fold basis. Firstly, a brief summary of repositories, methodologies, and codes is 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

1. Data Repositories

Up to 28 data repositories have been reported. In what follows, the name of the repository and a brief description as provided by the person who completely filled the information of the questionnaire is listed. In the map, this additional information is also provided:

- The name of the person who filled out 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
- 18 people are data providers actually
- 7 repositories are associated with the EERA Geothermal JP, 3 to NM, and 1 to Ocean, Wind, and DfE
- 19 repositories follow FAIR principles (there are 3 empty answers that could be potentially added to the previous number)
- 14 repositories count on metadata standards (a fact that could reduce the previous item, actually)
- 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 follow.

1. 4TU.ResearchData (TU DELFT)

To publish/archive research data underlying scientific publications.

2. CSP.guru (PSA)

This dataset holds technical, economic, financial, and industrial data from all operating concentrating solar power stations and stations under construction. It is periodically updated, the latest update dates to January 2023.

3. Dutch North Sea offshore wind measurements (TNO)

The data are collected over a period of almost 10 years from Lidar systems on offshore platforms in the North Sea. In addition, floating lidar campaigns are included. The data are collected to support the tender processes of the Dutch offshore wind farms.



4. e-cienciaDatos (CIEMAT)

To deposit the data of a scientific article.

5. EGRISE (CNR)

To collect and retrieve deliverables, articles, and products from EU geothermal-funded projects.

6. 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.

7. ENTENTE (CIEMAT)

European Database for Multiscale Modelling of Radiation Damage.

8. ERA5 (CIEMAT)

Source for meteorological data.

9. Geothermcatalog (CNR)

To catalogue Italian Geothermal datasets.

10. GFZ Data Services (GFZ POSTDAM)

Data archiving and publication, valid for assessing already published data.

11. Global Heat Flow Database (GFZ POSTDAM)

Compiling the IHFC compilation of the global heat flow data.

12. IEA PVPS Task 13 Data Base (AIT)

Performance, Operation and Reliability of Photovoltaic Systems.

13. IHFC Global Heat Flow Database (GFZ-Postdam)

To get access to the global compilation of heat flow data.

14. INESC TEC research data repository (INESC TEC)

Open data policy at INESC TEC.

15. International Criticality Safety Benchmark Evaluation Project – ICSBEP (CIEMAT)

Nuclear energy oriented research.

16. JANIS (CIEMAT)

Visualizing nuclear data for nuclear energy oriented research.

17. Materials project (UNIOVI)

Check on known systems to aid in computational materials design.

18. ODIN Portal (EUROPEAN COMMISSION)

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

19. Open Energy Platform (DLR)

Ontology, scenarios.

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20. Open Guided Waves (U. PERPIGNAN)
Training and testing machine learning models in order to detect, diagnose and localize structural flaws.
21. PED Labs UE (CIEMAT) COST ACTION PED UE NET
22. PetroPhysical Property Database P3 (TU DARMSTADT)
Reservoir rock characterization.
23. PVGIS (AIT - CIEMAT)
This data bank delivers PV performance and solar radiation data in the areas covered by Meteosat and GOES satellites and also provides tools running on this DB.
24. Repositório LNEG (LNEG)
Obtain references and read articles.
25. RISIS (AIT)
Analyses for Research & Innovation policies.
26. ViMiLabs (FZJ)
Materials discovery.

2. Methodologies

Up to 41 digital (AI) methodologies have been reported. In what follows, the name of the methodology and a brief description as provided by the person who completely filled in the information of the methodology is listed. In the map, this additional information is also provided:

- The name of the person who filled out 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 out 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:

- 18 methodologies are open source, being assumed that the rest can be jointly exploited by new groups under a collaboration scheme
- 24 methodologies have been developed by the proposing person



- The EERA Geothermal JP is exploiting 3 methodologies, NM is exploiting 2, and FCH JP is exploiting an additional one
- Some of the requirements associated with 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 follow.

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. CSP-AI (CNRS)
Machine/deep learning techniques combined with advanced automatic techniques, to control (concentrated) solar energy systems.
5. Drilling automatization (FRAUNHOFFER)
6. EOF, CCA and cluster analysis (CIEMAT)
Studies of variability, uncertainty, regionalization...
7. 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.
8. Energy time series forecasting toolbox (INESTEC)
R&D projects and software development for forecasting companies (technology transfer).
9. European Geothermal Research and Innovation Search Engine – EGRISE (CNR)
To retrieve products from EU geothermal-funded projects.
10. Flexible market (NORCER)
Multi-period Hybrid AC/DC-OPF Model for Flexibility Market Clearing with Seamless TSO-DSO-LEC Coordination.
11. Framework for Integrated Sustainability Assessment – FISA (CIEMAT)
Assessing sustainability indicators of energy investments.
12. Gamma spectrometry: Solver to adjust peaks in (CIEMAT)
Applications of VBA_excel (Visual Basic for applications) for calculating activity concentration and validating results for accreditation. Efforts to connect the computers to scales, alpha spectrometer and validation

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techniques. Methodology to add spectrum and to improve the sensitivity of methods and detection of radionuclides in air.

13. GeoStats (RWTH-AACHEN)

Spatial parameterisation, geostatistics and geological modeling with machine learning components for geothermal reservoir structures, as a basis for discussions and planning and as input for geothermal reservoir simulations.

14. 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.

15. Geothermal suitability by using MaxEnt machine learning algorithm (CNR)

Prediction of geographical suitability of geothermal power plants.

16. GETMORE (INPEN)

Assisted well-placement optimization.

17. Heat exchanger (UIS)

The data-driven machine learning methods are used to predict the performance of borehole heat exchangers for space heating and cooling purposes by means of recurrent neural networks for multivariant time series data.

18. Materials characterization (POLITO) Materials characterization

19. Materials science (UNIOVI)

Multipurpose tool for computational nuclear materials simulations.

20. Method and device for preserving the privacy of linear regression distributed learning (INESTEC)

21. Smart4RES EU project and software development for different use cases like forecasting and voltage control

22. 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).

23. Multiscale modelling of electrochemical data (DIFFER)

Multiscale modelling of electrochemical data.

24. Navier Stokes solver (CIEMAT)

Simulation of flames and reacting flows, simulation of heat transfer.

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

Smart meter data analytics.



26. Planning (LNEG)
Offshore planning.

27. Reduced Graphene Oxide Synthesis (CIEMAT)
The methodology provides graphene materials for different projects related to the development of sulphur gas adsorbents, solar cells, hydrogen storage and supercapacitors.

28. SiteAdapt (CENER)
Improvement of the accuracy of estimated solar radiation datasets, like satellite-based time series for a particular location taking into account their specific characteristics. The obtained site-adapted time series could be used to perform solar energy system simulations using high spatial resolution solar resource data.

29. Solar Collectors (PSA)
Neural network for improving the control of solar collectors.

30. Solar Radiation (CENER)
Methodology for increasing the temporal resolution of solar radiation datasets for accurate simulations of the performance of solar energy systems, especially photovoltaic.

31. Stata econometrics (UCD)

32. StockFlow (DLR)
Consistent modeling framework and user interface based on post-Keynesian macroeconomic modeling and energy system transitions.

33. TELLUS (IFPEN)
A multi-purpose tool focused on knowledge mining in massive collections of geoscience documents, interactive forecasting of production and physical variables at well locations with time series analysis and Machine Learning, accelerated interpretation of logs, core and thin sections with Machine Learning.

34. TMY (CENER)
Typical Meteorological Year (TMY) generate a yearly time series representative of a particular location and different levels of available solar resources corresponding to a predefined probability of exceedance. These time series could be used as input data for solar energy systems simulation activities.

35. Tensorflow (VTT)
Flaw detection in ultrasonic data.

3. Numerical codes

Up to 83 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 in the information of the code are listed. In the map, this additional information is also provided:

- The name of the person who filled out the survey
- His/her e-mail address for potential contacts
- The name of the code

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methodologies, and numerical codes

- If it is open source
- If the person who filled out 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:

- 36 codes are open source, being assumed that the rest can be jointly exploited
- 37 codes have been developed by the proposing person
- 16 Codes are being exploited under the EERA Geothermal (8), AMPEA (2), ESI (2), E3S (1), NM (3), Smart Grids (1), and Wind (1) JPs
- Most of the codes are run in a Linux-based environment

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

1. ABAQUS (EUROPEAN COMMISSION)

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. AMIRIS (DLR)

Evaluation of future energy markets, their market design, and energy-related policy instruments, including electricity prices.

5. ANSYS-CFX / ANSYS-FLUENT / ANSYS-ICEMCFD / ZView (U. SEVILLA - CIEMAT)

ANSYS-CFX: Computational Fluid Dynamics modelling and simulation. For performing CFD calculations mainly focused on MHD and buoyancy interaction in PbLi flows inside fusion breeding blankets.

6. ASCOT (CIEMAT)

Simulations of fast-ion confinement in magnetically confined fusion devices.

7. ASTEC (CIEMAT)

Numerical simulations for severe accident phenomena in nuclear power plants.

8. ComPASS (BRGM)

Hydrothermal modelling.



9. CRESCENDO (CEA)

Cluster dynamics simulation of diffusion in nuclear fuels.

10. 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 detail, 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.

11. CRITIC2 (BRGM)

Hydrothermal modelling.

12. DYMOKA (U. LILLE) MD simulations.

13. Ecosim (CIEMAT)

Tritium breeding blanket modelling and simulations.

14. EES (LNEG)

Modelling and simulation of thermodynamic systems (power cycles, absorption chillers, etc.).

15. EnergyBox (IREC)

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

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

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

Supercapacitors, flywheels, 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).

18. EUTERPE (CIEMAT)

Gyrokinetic simulations of plasma turbulence in stellarators.

19. EVOLCODE (CIEMAT)

Calculation of isotopic evolution of nuclear reactors.

20. FAME (DLR)

Open Framework for distributed Agent-based Models of Energy systems.

21. FHI-AIMS (CSIC)

To compute energies of solids and molecules.

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22. FRAPCON (CIEMAT)

For research on fuel thermo-mechanical performance.

23. FRAPTRAN (CIEMAT)

For research on fuel thermo-mechanical performance under transient conditions.

24. 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.

25. GIBB2 (U. Oviedo)

Calculation of thermodynamic properties of solids in the quasiharmonic approximation.

26. 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.

27. GridapMHD (CIEMAT)

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

28. HOMER Pro (CIEMAT)

Analysis and design of renewable energy systems.

29. KINECLUE (CEA)

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

30. KNOSOS (CIEMAT)

Numerical calculation of transport in fusion plasmas.

31. IOG2X (DLR)

Model coupling optimization models with agent-based simulation models.

32. 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.

33. Libradtran (CIEMAT)

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

34. MCNP (CIEMAT)

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



35. MELCOR (CIEMAT)

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

36. MODELICA-CST (CENER)

CENER's in-house Modelica library that allows the simulation of components like solar collectors, receivers, as well as solar systems for power generation (CSP), process heat supply, and energy storage.

37. 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).

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

39. 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.

40. NJOY (CIEMAT)

Nuclear data processing for nuclear-energy oriented research.

41. 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.

42. OPenFOAM (CIEMAT)

3 dimensional simulations of combustion problems.

43. OpenFoam (CENER)

Wind turbine aerodynamic computations, and wind turbine platform hydrodynamic computations.

44. Optica (CIEMAT)

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

45. PENELOPE (CIEMAT)

Simulation ionizing radiation detector.

46. Phonons Monte Carlo (U. LORRAINE)

Computing thermal transport properties of semiconductors.

47. PLATOON (CIEMAT)

Thermal-hydraulic modelling at system level in fusion breeding blankets.

48. PorePy (UIB)

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

49. 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.

50. Q2DHS (CIEMAT)

Flame dynamics calculation in a Hele-Shaw cell configuration.

51. 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.

52. SCALE (CIEMAT)

Nuclear energy-oriented research.

53. SERPENT (CIEMAT)

Particle transport calculations for nuclear energy oriented research.

54. 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.

55. SILVACO-ATLAS (CENER)

Modelling of the electro-optical behaviour of solar cells.

56. SIM-PV (CENER)

Performance of either alone or integrated PV systems without restrictions on their configuration or composition.

57. 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.

58. SOLTrace (LNEG)

Optical simulation of concentrating solar collectors.

59. Stella (CIEMAT)

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



60. STELLOPT (CIEMAT)
Optimization of stellarator configurations.

61. System Advisory Model (LNEG)
Simulation of CSP power plants.

62. TIMES (CIEMAT)
Energy systems optimization.

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

64. Tonatihu (CENER, LNEG)
Design, simulation, analysis, and optimization of the optical performance of any concentration solar system.

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

66. TRNSYS (LNEG)
Transient simulation of energy systems. Current work focuses mostly on solar thermal systems and applications (solar thermal electricity, solar heat for industrial processes, solar heating and cooling) but the software can be used to simulate other energy systems (PV, CHP, etc.).

67. VASP 6.x (CEA, CSIC, UNIOVI)
Electronic structure calculations on nuclear fuels and structural nuclear materials. Also, computing structures and energies of different solids ($\text{CuO}_x/\text{CeO}_2$, interfaces between semiconductors and photocatalysts (Ce,ZrO_2 , etc.).

68. VITALITY Plugin, within Grasshopper / Rhino environment (AIT)
Tool for the optimized placing of PV panels within the building envelope, considering (local) solar resources 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.

1. 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

2. Geothermal / Ocean / Wind

Repositories

- EGRISE (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
- IHFC Global Heat Flow Database (GFZ-Postdam)
To get access to the global compilation of heat flow data
- PetroPhysical Property Database P3 (TU DARMSTADT)
Reservoir rock characterization

Methodologies

- Drilling automatization (FRAUNHOFER)
Drilling processes
- 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
- Geothermal suitability by using MaxEnt machine learning algorithm (CNR)
Prediction of geographical suitability of geothermal power plants
- GeoStats (RWTH-AACHEN)
Spatial parameterisation, geostatistics and geological modeling with machine learning components for geothermal reservoirs structures, as basis for discussions and planning and as input for geothermal reservoir simulations
- 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
- 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

3. 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.)

4. 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 detail, 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
- MODELICA-CST (CENER)
This CENER's in-house Modelica library allows the simulation of components like solar collectors, receivers, as well as solar systems for power generation (CSP), process heat supply, and energy storage

- **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
- **SOLTrace (LNEG)**
Optical simulation of concentrating solar collectors
- **System Advisory Model (LNEG)**
Simulation of CSP power plants
- **Tonatiuh (CENER, LNEG)**
Design, simulation, analysis, and optimization of the optical performance of any concentration solar system
- **TRNSYS (LNEG)**
Transient simulation of energy systems. Current work focuses mostly on solar thermal systems and applications (solar thermal electricity, solar heat for industrial processes, solar heating and cooling) but the software can be used to simulate other energy systems (PV, CHP, etc.)
- **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

5. AMPEA / Nuclear Materials

Repositories

- **ENTENTE (CIEMAT)**
European Database for Multiscale Modelling of Radiation Damage
- **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)

Codes

- Materials characterization Materials science (UNIOVI)
Multipurpose tool for computational nuclear materials simulations
- ABAQUS (EUROPEAN COMMISSION)
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

6. 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 EERAdataproject)
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

7. Bioenergy / Carbon Capture and Storage

Methodologies

- Gamma spectrometry: Solver to adjust peaks (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.



Codes

- Multiscale modelling of electrochemical data (DIFFER)
Multiscale modelling of electrochemical data

8. 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)

9. 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

10. 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

11. (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 scenario

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