Materials characterisation challenges to support the industry transition in the digital era

MODA and CHADA; challenges and opportunities for integration and exploitation to industrial stakeholders beyond EU projects.

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[3] QWED, Poland. H2020 NanoBat

nanoMECommons Co-Creation Workshop
13 December 2021

Background and Motivation

- Materials Modelling status 10 years ago
  - Multiple Communities
  - Multiple Terminologies
  - No agreed classification or way of documentation
- Materials Characterisation
  - Same state
- Increasing industrial use and expected maturity
  - Need for standards in documentation and interoperability
  - FAIR data

Typical materials model descriptions …

- By **phenomena (application)**:
  - "I have a mikro-kinetics model."
- By **scale** of the phenomena:
  - "I have a mesoscale model."
- By name of the **software (code)**
  - "I use the Uppsala model"
- By **solver**:
  - "I have a FE model"

Objectives and Benefits

- Communication tool: capture and convey application of modelling and characterization
  - To wider audience of scientists and engineers
  - Complex characterisation or modelling process shown "in a nutshell", visible "at a glance“
- Standard documentation
- Potential to use in Data Management and as Supplementary Material in Publications: standardized form means better quality control
- Widely agreed terminology and classification a first step to digitalisation

EMMC activities on MODA

2015: EMMC works on MODA

MODA - Description & use cases

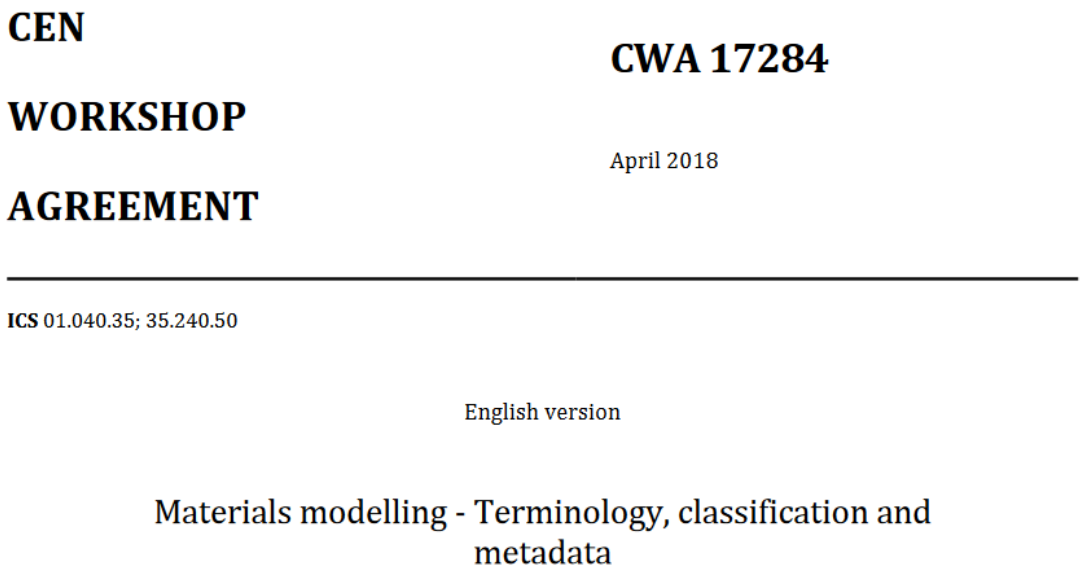
MOdelling DAta

In a CEN Workshop Agreement, CWA 17284 "Materials modelling - terminology, classification and metadata", several stakeholders formally agreed on:

Terminology used to describe materials modelling

https://emmc.eu/moda/

2018: EMMC CEN/CWA 17284



CEN

WORKSHOP

AGREEMENT

CWA 17284

April 2018

ICS 01.040.35; 35.240.50

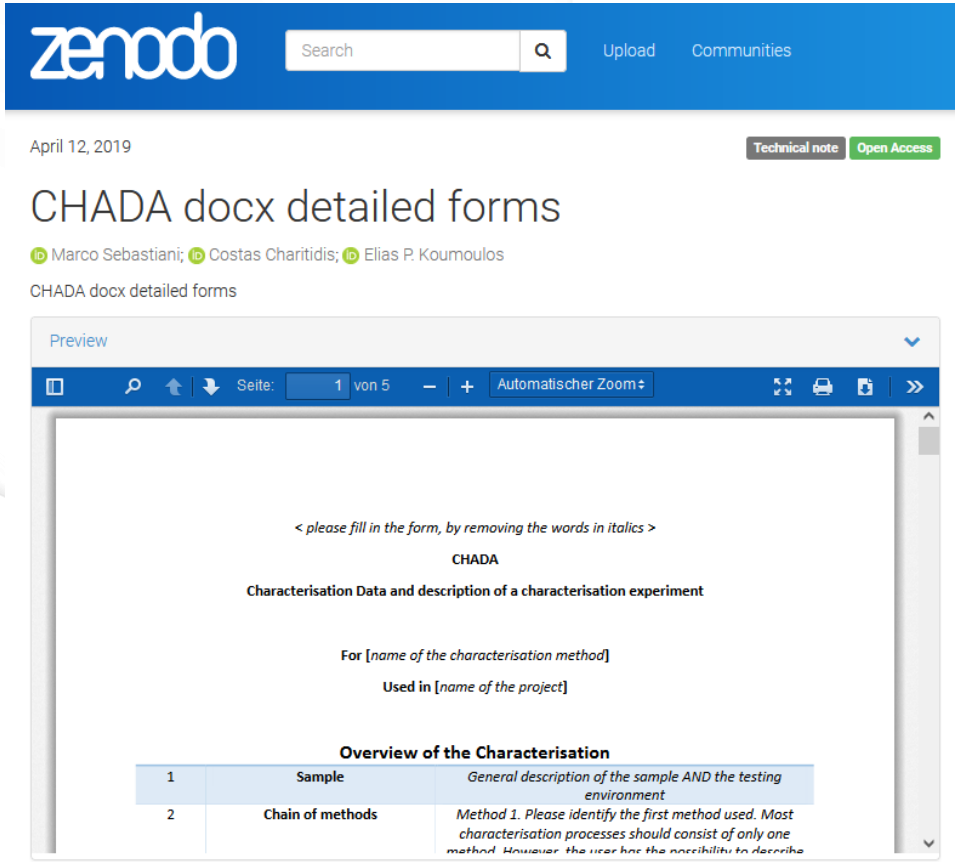
English version

Materials modelling - Terminology, classification and metadata

https://emmc.info/wp-content/uploads/2018/05/CWA_17284.pdf

EMCC activities on CHADA

2019: EMCC works on CHADA



https://zenodo.org/record/2637419#.YbMXUyYxm9I

2021: CEN/WS 'OYSTER on Materials characterisation - Terminology, classification and metadata'

The Workshop and the related CWA provide standardised terminology that will improve future exchanges among experts in the entire area of materials characterisation, facilitate the exchange with industrial end-users and experimentalists and reduce the barrier to utilising advanced materials characterisation.

The common language is expected to foster dialogue and mutual understanding between industrial end-users, equipment manufacturers, and academic researchers. Standardisation of terminology and classification has been identified as critical to collaboration in and dissemination of European research projects. In particular, standards will facilitate interoperability between methods and databases. The standardization is relevant for an integrated technological development and brings benefits for industrial end-users due to simplified and much more efficient communication in the field of materials characterisation. The classification helps data interpreters by translating industrial problems into problems that can be analysed with characterisation methods. It assists workflow development where several methods can interoperate in addressing a specific end-user question.

- Draft CWA 'Materials characterisation - Terminology, classification, and metadata' (pdf)
- Commenting form (word)
- Project Plan (pdf)

https://www.cencenelec.eu/news-and-events/news/2021/workshop/2021-06-23-cen-ws-oyster-materials-characterisation/

EuroNanoForum 2019

Collaboration of EMMC and EMCC

June 12-14, 2019, Bucharest, Romania

An event of the Romanian Presidency of the Council of the European Union

EuroNanoForum 2019

HOME PROGRAMME SPEAKERS EXHIBITION INFORMATION MEDIA AFTER EVENT

MODA and CHADA: Terminology and standardized documentation for materials modelling and characterisation

Alexandra Simperler, Gerhard Goldbeck, Goldbeck Consulting Ltd

Marco Sebastiani
Università degli studi Roma TRE and EMCC

https://emmc.info/wp-content/uploads/2019/06/Euronano2019-MODA_CHADA_final.pdf

Horizon Europe: contributions EMMC & EMCC

2020 : Input for the work programme Horizon Europe in empowering the cooperation between materials' characterisation and materials' modelling.

This is well reflected in both RoadMaps.

Topic title: Advanced materials modelling and characterisation

Expected outcomes: To increase the efficiency and effectiveness of materials and product development by creating a digital continuum including materials modelling (data and physics based as well as engineering modelling), characterisation (material properties/functionalities) and safety, all supported by artificial intelligence or machine learning.

Scope: The action should investigate the development of advanced materials by rational design, with focus on the combination of theory with large-scale computational screening (e.g. Artificial Intelligence or Machine Learning). The validation by experimental methods should be included. The action should cover domains of the Green Deal Strategy (e.g. decarbonising industries or sustainable materials).

Working Groups

WG 3 Characterisation Data and Information Management.

WG 3.1 MODA & CHADA interaction with EMMC.

EMMC International Workshop 2021

Towards pairing up materials modelling and characterisation

3rd EMMC International Workshop
March 4th 2021

Javier Sanfélix & Yanaris Ortega Garcia – Project and Policy Officers

DG Research&Innovation – Unit F4 "Materials for Tomorrow"

European Commission

Javier Sanfelix

Yanaris Ortega Garcia

https://www.youtube.com/watch?v=jihszf4FD3o

EuroNanoForum 2021

Collaboration of EMMC and EMCC

Advanced materials modelling and characterisation: strategies for integration and interoperability

Date: 04.05.2021 - 04.05.2021
Organisers: ENF Satellite Event organised by EMMC & EMCC
Venue: ENF 2021 Virtual Arena

EuroNanoForum - ENF is the major European Conference on Nanotechnology, hence a unique opportunity for reaching out to the European and International community of Nanotechnology and Advanced Materials.

On **May 4**, a day before the inauguration of the conference, **ENF promotes a set of satellite events**.

In this workshop, some current activities regarding interoperability and integration will be presented. In particular, EMMO, MODA and CHADA will be discussed to highlight their usability and utility as a basis for moderated discussions related to the above Topics.

EuroNanoForum 2021

European Materials Modelling Council

European Materials Characterisation Council

Report on Advanced materials modelling and characterisation: strategies for integration and interoperability

EuroNanoForum 2021 Satellite Event, 4th May 2021

Published in June 2021

DOI:10.5281/zenodo.4912683

https://zenodo.org/record/4912683#.YbH2USYxm9I

HORIZON EUROPE

Advanced materials modelling and characterisation (RIA)

TOPIC ID: HORIZON-CL4-2022-RESILIENCE-01-19

Programme

Horizon Europe Framework Programme (HORIZON)

Call

A DIGITISED, RESOURCE-EFFICIENT AND RESILIENT INDUSTRY 2022 (HORIZON-CL4-2022-RESILIENCE-01)

Type of action

HORIZON-RIA HORIZON Research and Innovation Actions

Opening date

12 October 2021

Deadline date

30 March 2022 17:00:00 Brussels time

EMMC Brokerage Event

EMMC Horizon Europe Cluster 4&5 Consortium Brokerage Event

Date: 01.10.2021 - 01.10.2021
Organisers: EMMC
Venue: AIRMEET / Online

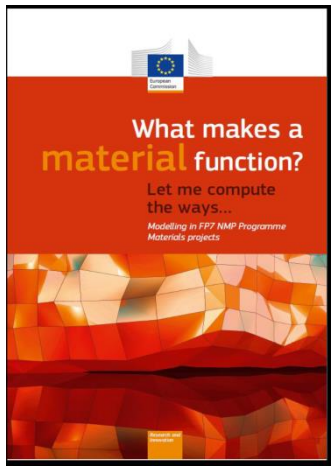
Agenda

- Introduction (Nadja Adamovic, Gerhard Goldbeck)
- Topic Advanced Materials Modelling and Characterisation (RIA) (Overview by Javier Sanfelix, EC)
- Project Idea Pitches (10 minutes each)
- Individual Project discussions at tables in the Airmeet platform

Review of Materials Modelling (RoMM)

- Catalogue EU projects involving materials modelling
- Foster **dialogue** and mutual **understanding** between industrial end-users, software developers and theoreticians.
- Establish a **terminology** for materials modelling concepts harmonising the language of subfields.
- Definition of **concepts**, **classification**
- Basic **metadata** for describing modelling

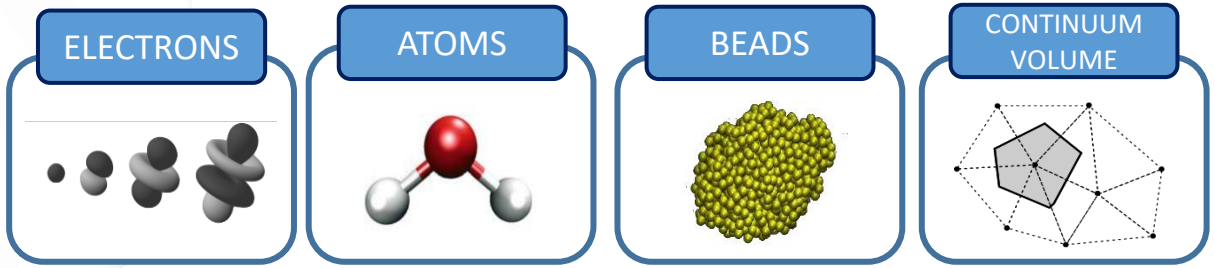
a compendium of >100 projects and classification/terminology of materials modelling



http://ec.europa.eu/research/industrial_technologies/modelling-materials_en.html

CEN Workshop Agreement (CWA): materials modelling - terminology, classification and metadata

- **Terminology used to describe materials modelling**
- **Classification of materials models**
  - **Taxonomy based on entity (4), physics equation (24), materials relation (1000s)**



- **Standardised documentation of Simulations (MODA)**

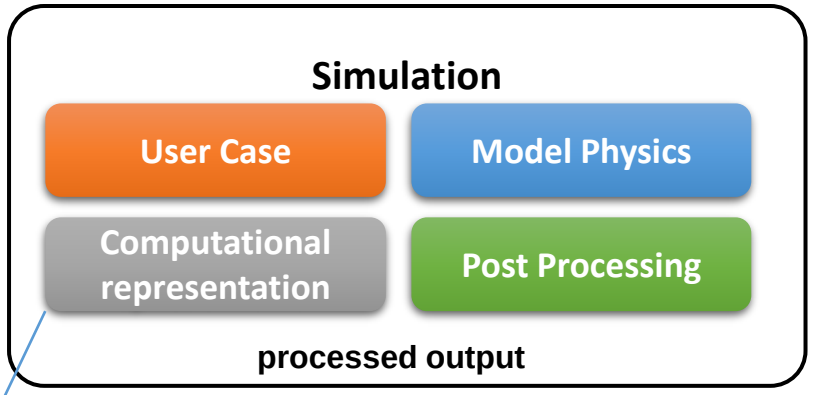
MODENA
GA604271

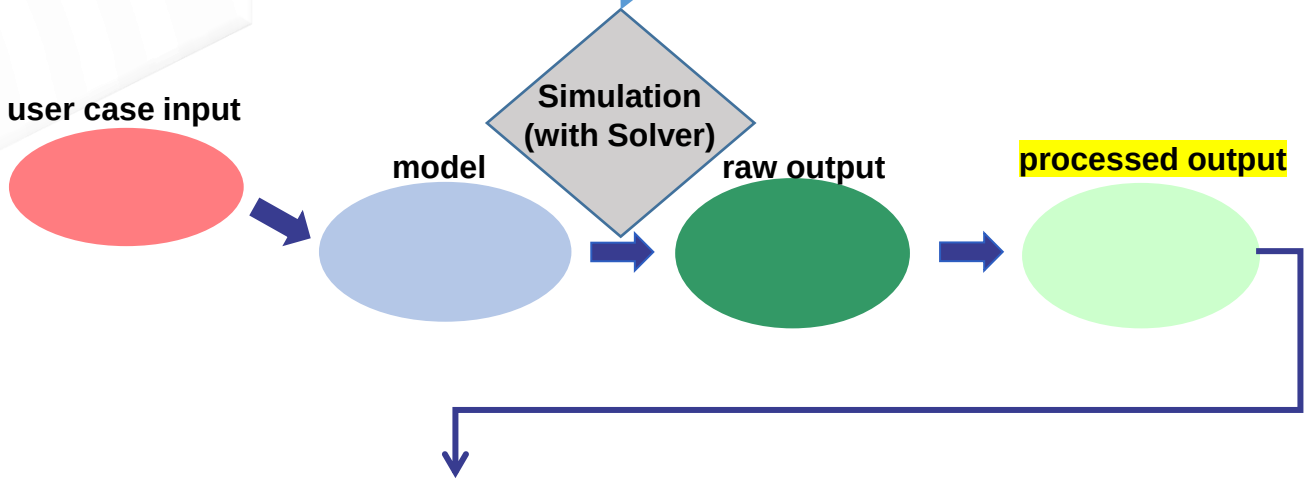
CWA 17284 "Materials modelling - terminology, classification and metadata"

https://www.cencenelec.eu/media/CEN-CENELEC/CWAs/RI/cwa17284_2018.pdf

Standardised documentation (MODA)

A common language and formal approach how to log a simulation project



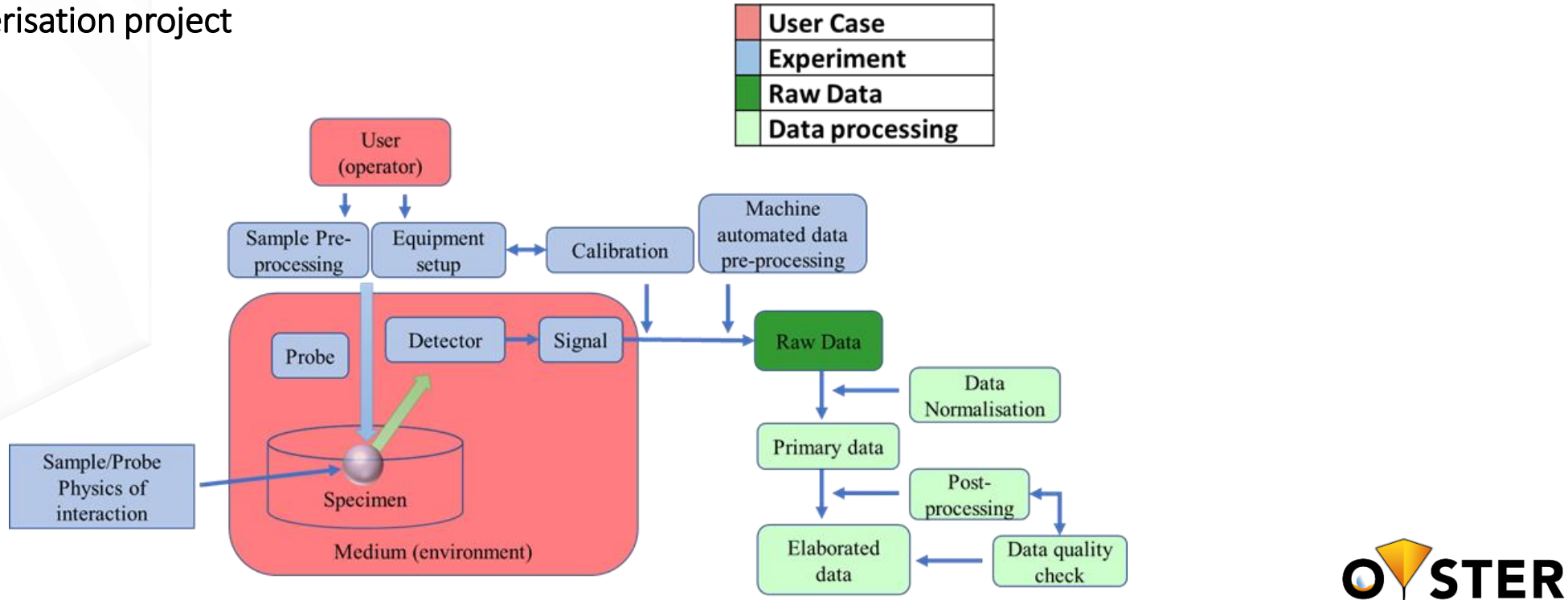


MODA for <user-case>
***Simulated* in project <acronym>**

	OVERVIEW of the SIMULATION		
1	User Case		*General description of the User Case.* *Please give the properties and behaviour of the particular material, manufacturing process and/or in-service-behaviour to be simulated. No information on the modelling should appear here. The idea is that this user-case can also be simulated by others with other models and that the results can then be compared.*
2	Chain of Models	Model 1	*Please identify the first model. Note these are assumed to be physics-based models unless it is specified differently.* *Most modelling projects consist of a chain of models, (workflow). Here only the Physics Equations should be given and only names appearing in the content list of the Review of Materials Modelling VI should be entered. This review is available on http://cc.europa.eu/research/industrial_technologies/e-library.cfm) All models should be identified as electronic, atomistic, mesoscopic or continuum.*
		Model 2	*Please identify the second model.*
		Data-based model	*If data-based models are used, please specify.*
3	Publication Peer-Reviewing the data		*Please give the publication which documents the data of this CINE simulation.* *This article should ensure the quality of this data set (and not only the quality of the models).*
4	Access conditions		*Please list whether the model and/or data are free, commercial or open source. Please list the owner and the name of the software or database (include a web link if available).*
5	Workflow and its rationale		*Please give a textual rationale of why you as a modeller have chosen these models and this workflow, knowing other modellers would simulate the same end-user case differently.* *This should include the reason why a particular aspect of the user case is to be simulated with a particular model.*

Standardised documentation (CHADA)

A common language and formal approach
how to log a characterisation project



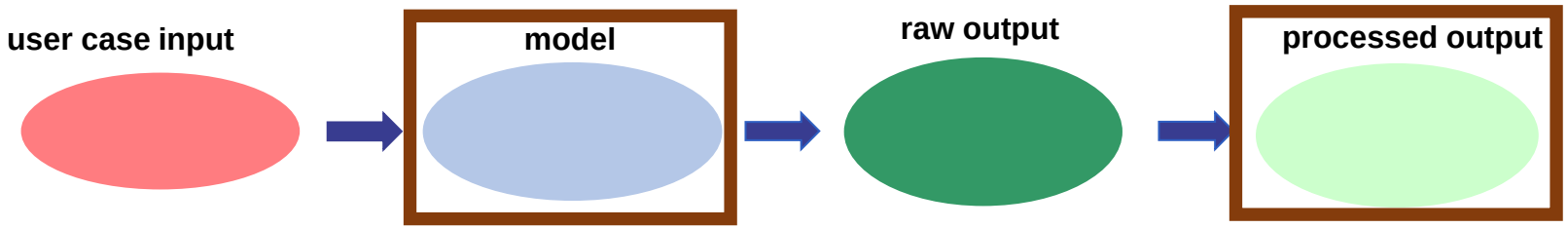
CWA 17815 "Materials characterisation - Terminology, metadata and classification "

https://www.cencenelec.eu/media/CEN-CENELEC/CWAs/ICT/cwa17815.pdf

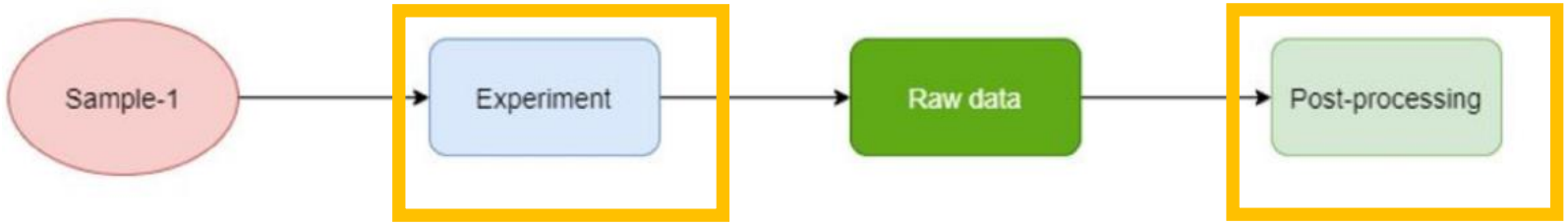
MODA vs CHADA overview

- Similar approach & colours, so compatibility can be expected

MODA from slide 16



CHADA from CWA 17815:2021



- ...but MODA & CHADA are inconsistent in the capturing of

DATA / STATE versus OPERATION / PROCESS

Note:
"experiment" corresponds to "simulation"
"model" is more like and "experiment design"
"processed output" is a results of "post-processing"

Advantages

- Twinning MODAs + CHADAs will enhance the development of both MODELLING and CHARACTERISATION
- Ideally:
  - each tangible element of a CHADA will have its digital twin

  in the form of a data set on a computer
  - each physical process in an experiment will have its digital twin

  in the form of an executable computer algorithm

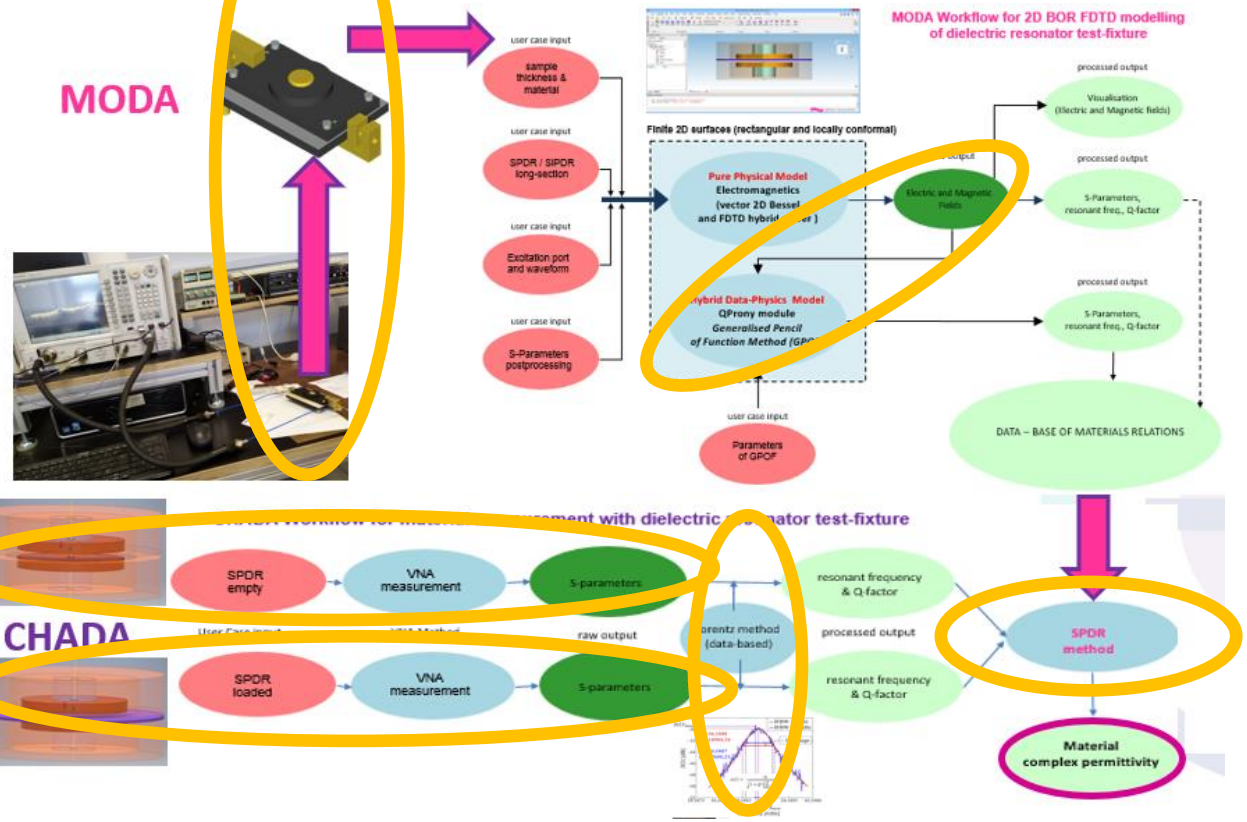
The **twinning of MODA+CHADA** has been demonstrated and even used in industry but full synergies are still to be exploited.

Twinned MODA + CHADA Example

Electrical characterisation in GHz frequency range:

- microwave measurement (resonant test-fixture + with network + PC app
- electromagnetic modelling with FDTD method

10 units/ months, recognised as EU H2020 Innovation Radar



1. CHADA is often a set of CHADAs (parallel, sequential, or linked)
2. Completing CHADA typically requires input from MODA (often unconscious)
3. MODA emulates CHADA on a computer
4. POSTPROCESSING is actually MODELLING; so a MODA with postprocessing is actually a set of linked MODAs
5. TWINNING enhances the PHYSICAL UNDERSTANDING

What comes next – at a glance

OBJECTIVES:

- enhance research collaborations,
- encourage industry to use research results,
- enhance European excellence, competitiveness, wellbeing

OPPORTUNITIES:

- standardised data facilitate collaborations,
- MODA & CHADA are ”visual” – appealing to end-user
- effective & efficient information flow, quality control, shorter time-to-market

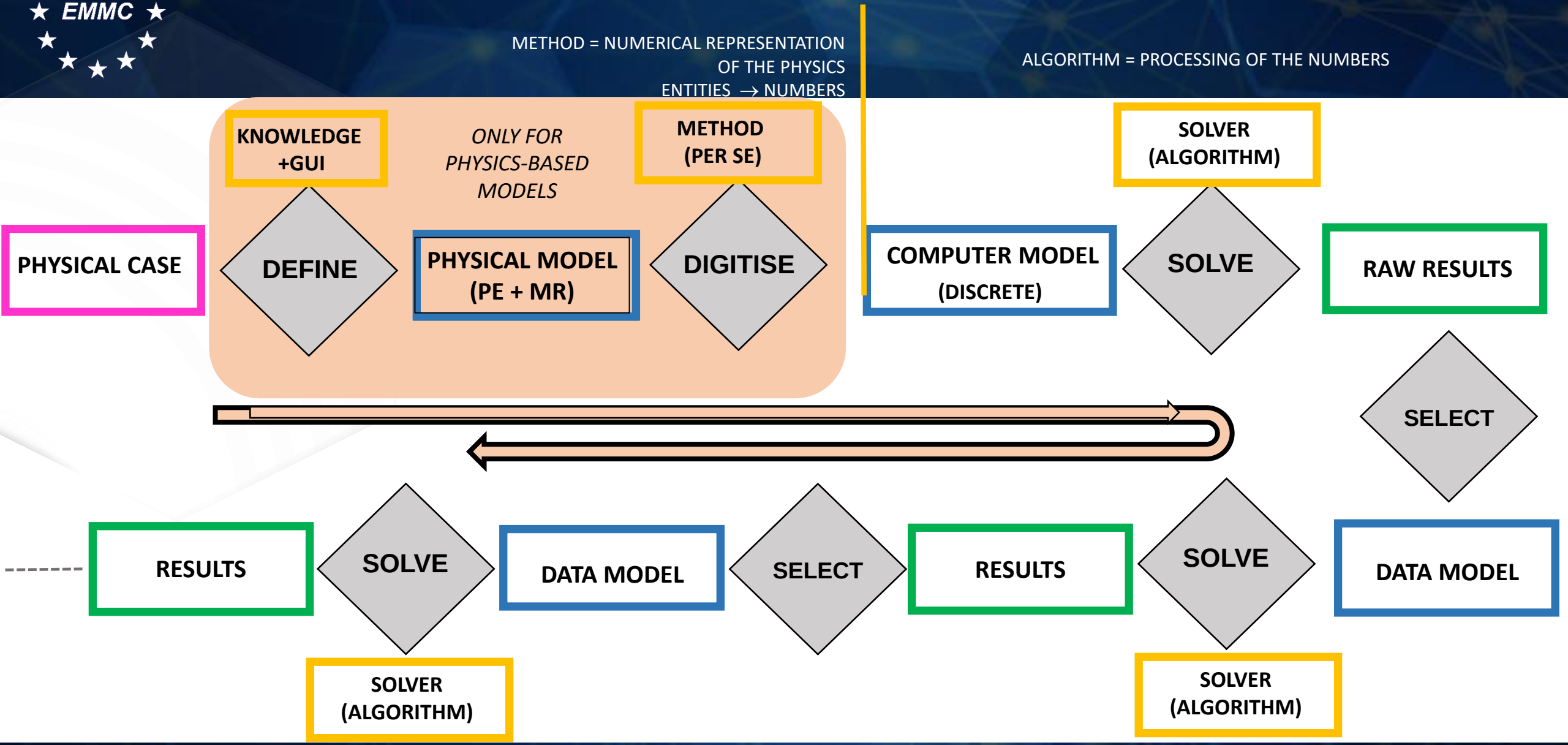
CHALLENGES:

- pre-established working habits…
- time & training needed to develop & use documentation
- large accumulated heuristic knowledge and data repositories in diverse formats

ACTIONS:

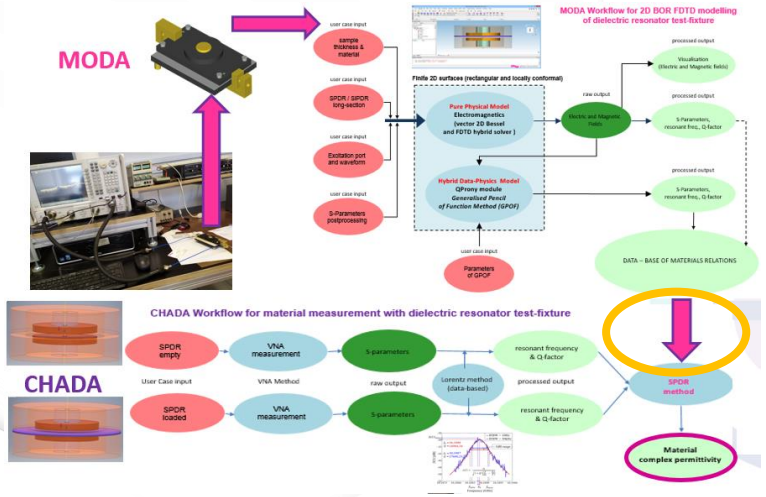
- **SIMPLIFY**
- **UNIFY**
- **AUTOMATE**
- **DISSEMINATE, COMMUNICATE, EDUCATE, EXPLOIT**

A generalised MODA structure

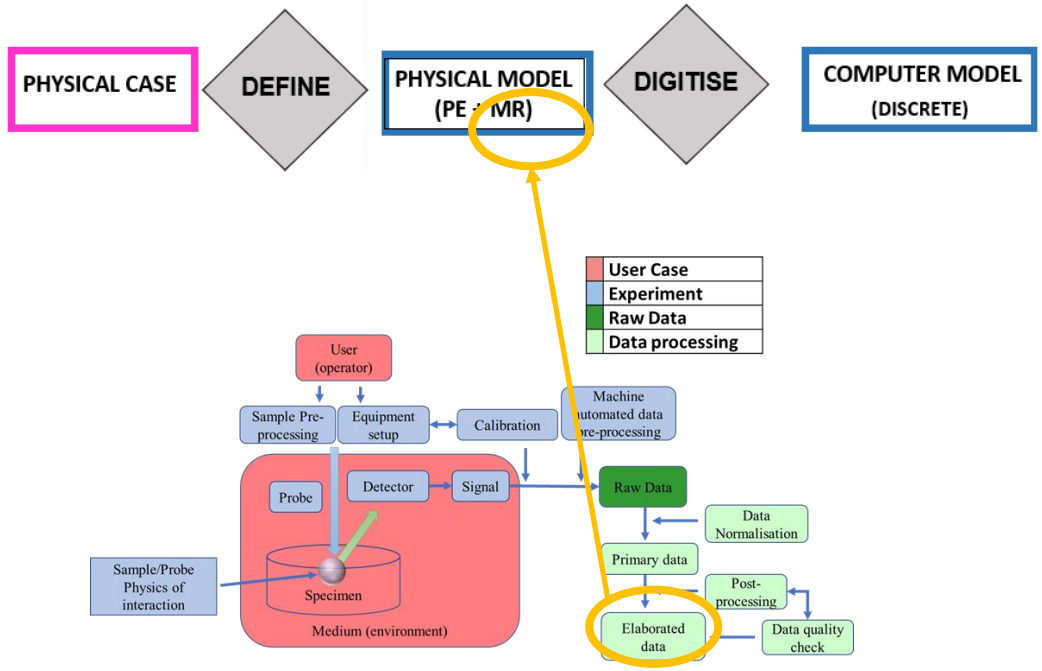


Generalised relations between MODA & CHADA

1. CHADA needs input from MODA



2. MODA needs input from CHADA



3. a chain (network) of MODAs & CHADAs solves the User Case

Challenges: mainly usability

Online MODA tool prototype

- Variability in interpretation
  - definitions not sharp enough
  - lack of classification and agreed taxonomies (apart from models)
- Time consuming to fill in
  - lack of online tools
  - not machine readable
- Not enough detail for some experts and too much for end users

Opportunities

- Standards for publication of modelling and characterisation
- Improved integration of characterisation and modelling
  - Modelling and characterisation as knowledge generators, e.g. for determining a property
  - Modelling of the characterisation- Characterisation as input to modelling
  - Validation
- Foundation for machine interoperable data documentation of modelling and characterisation
  - From electronic to digital: implementation in data systems, metadata schema and ontology based.
  - Link to workflow capture
  - Basis for industrial data documentation (lab informatics, knowledge capture)
  - Basis for collaboration, co-innovation, open innovation systems
- Improved communication and collaboration

Potential Extensions and Modification

- Extend to include equipment specs and whether you are willing to make your equipment available (access rights)
- Extend to comment on the necessary operator qualifications (technician, engineer, undergraduate, postgraduate, professional)
- Further develop some sections, e.g. post-processing in MODA…

BUT MAINLY:

- Simplify
- Unify
- Remove ambiguities

Potential Actions

- Initiate and encourage the development of MODA & CHADA libraries.
- Disseminate & teach: academic courses on the standards for documentation.
- Promote MODA&CHADA, and EMMC & EMCC, beyond the materials' research community - into the communities that USE rather than DEVELOP materials.
  - MODA & CHADA should help understand the quality (reliability, repeatability) of the materials' data & performance delivered with them (or by the characterising entity).
- Promote MODA+CHADA in industry (beyond the EU projects) and assembling success stories
- EU-funded research teams at universities and companies, when doing commercial consulting for industry, should aim to document their results in MODA & CHADA, to make industry acquainted with this way of documentation.
- Involve publishers and journals to establish MODA/CHADA as standard for supplementary information.

Key points for Discussion

- Improvements to CHADA and MODA
  - Clear distinction between Objects (Data/States) and Process (Actions)
  - Further review of definitions to ensure all are logical and consistent also across MODA and CHADA
  - Review all sections, and add more detail where needed
- Integrated CHADA-MODA system: new CWA?
- Online versions
  - Easier to fill in
  - Classification and Taxonomies: “pull down menus”
  - Different levels of granularity, depending on user

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