



## Simulation Documentation With Materials Modelling Data Tables



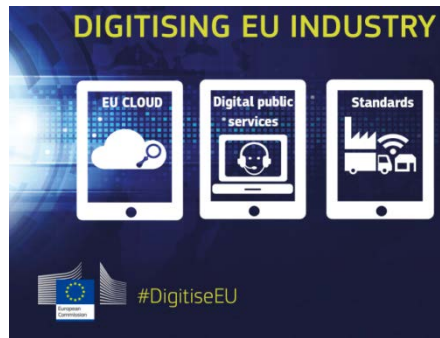
European Materials Modeling Council (EMMC)

<http://emmc.info>

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- The digitalization of European industry **necessitates integrating materials modelling** more deeply into the value chain of product manufacturing and development.
- Materials Modelling Marketplaces brings DSM to materials modelling → **requires enhanced curation schemes for materials modelling in general and documentation in particular** (see also talk by Welch Leite Cavalcanti today).
  - We use computers for modelling, but do not always provide a **„digital, machine processable,** documentation of our modelling“



<https://ec.europa.eu/digital-single-market/en/%20european-cloud-initiative>

(<https://ec.europa.eu/digital-single-market/en/digitising-european-industry>).



# The European Materials Modelling Council

## Intermezzo on Digitalisation, Big Data and Curation



- **Data curation** is a broad term used to indicate processes and activities related to the **organization** and **integration** of data collected from various sources, **annotation of the data**, and **publication** and **presentation** of the data such that the **value** of the data is **maintained over time**,
  - Data available for reuse and preservation.
- Data curation includes "all the processes needed for principled and **controlled data** creation, maintenance, and **management**, together with the capacity to add value to data
- In science, data curation may indicate the process of extraction of important information from scientific texts, such as research articles by experts, to be converted into an **electronic format**
- In broad terms, curation means a range of activities and processes done to create, manage, maintain, and **validate** a component



WIKIPEDIA  
The Free Encyclopedia



- Visibility:
  - Make your work more visible and discoverable
- Discoverability:
  - Enable non-modelling experts to discover quickly what modelling can do, including applications, users case, errors, etc.
  - Collaboration: Supports collaborations between experimentalist, translators and modellers.
- Curation:
  - Allow enhanced collaboration and reuse of modelling software.
- Documentation
  - Great for Students, R&D, modellers etc to communicate
- Publication
  - Still to come: DOIs for MODA, MODA as supplementary material.



# The European Materials Modelling Council

## State of the art



- Based on Microsoft Word files
  - Cumbersome to fill and extend beyond 1-2 models
  - Hard to curate, not properly “digitalised”
  - Can easily be “abused” in terms of formatting
  - Does not guarantee standard input of information
- The materials modelling community asked for an online tool!



- **Develop MODA online form for easy compilation, catalogue and formatting.**
  - Distinguish between free text field entries (e.g. description) and fixed options (e.g. model entities)
  - Provide standard PE for the 24 model types so that every applicant will not need to reinvent the wheel
  - Provide a first set of standard MR for the most common models
  -
- **Provide a navigable selected set of MODA examples** (from RoMM VI) for different fields of applications to be used as reference point
- Develop formal taxonomy and ontology

Slide from Dr. Anne F de Baas, EC



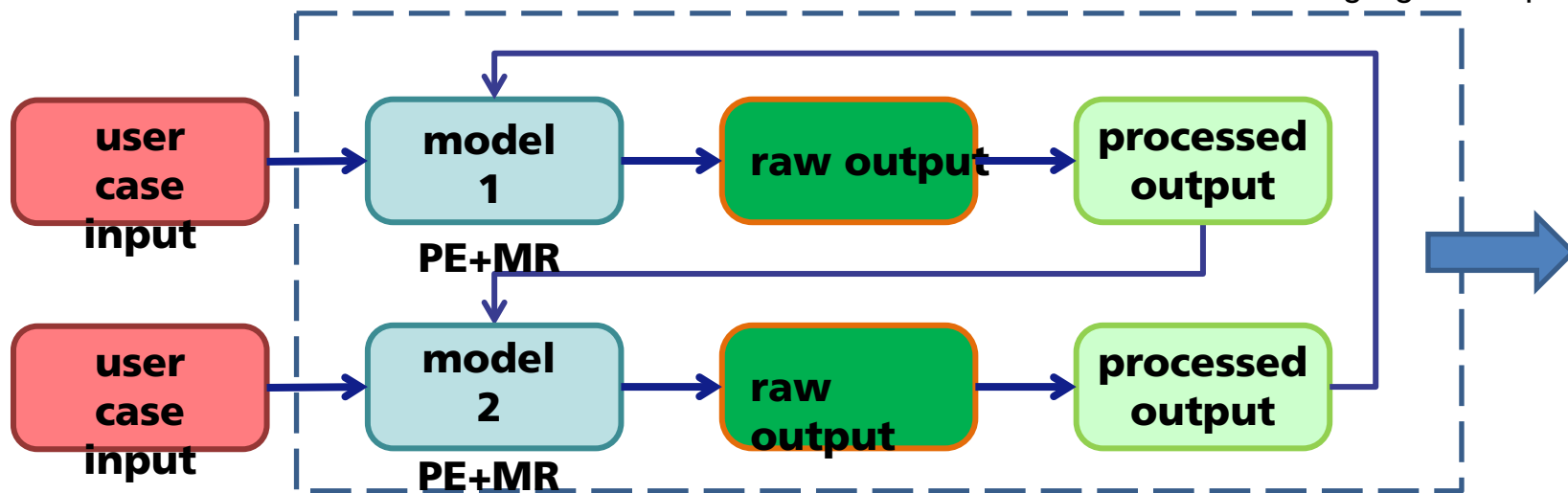
# The European Materials Modelling Council Requirements



- Easy to use
- Help make the right choices
  - controlled choice of models, physics equations and materials relations according to the RoMM, CWA and EMMO!
- Ensures adhering to one standard
  - ensures consistency with the EMMO as it is being developed
- Searchable
- Reviewing process
- Reliable!
- Available on-line!

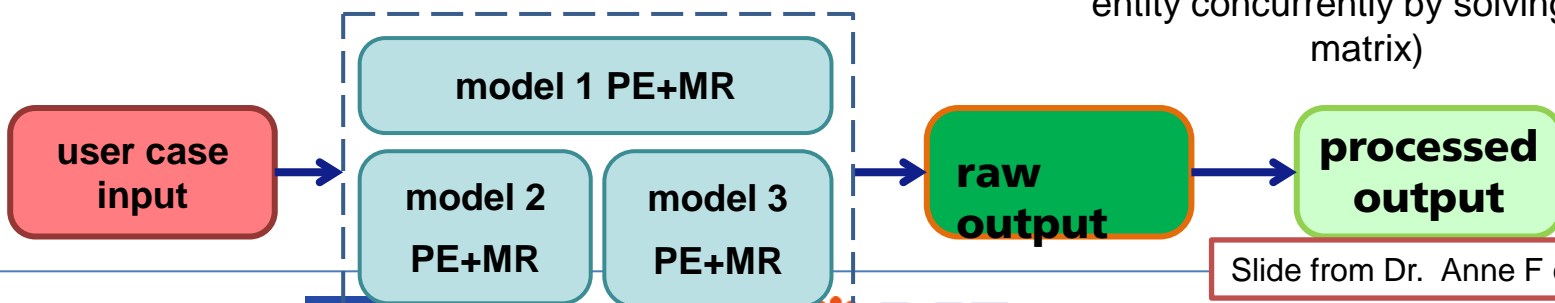
## workflow for an iterative chain

Iterative solution of segregated equations



## workflow for tightly coupled models

equations solved together  
(running different models for the same entity concurrently by solving one matrix)



Slide from Dr. Anne F de Baas, EC



Slide from Dr. Anne F de Baas, EC

PHYSICS-BASED MODEL

PHYSICS EQUATION  
**PE**

Equation based on a physics/chemistry theory which describes the spatial and temporal evolution of physics quantities of the entity

PHYSICS QUANTITIES

MATERIAL RELATIONS  
**MR**

Information on the material needed to close the PE and to make the system of Governing Equations solvable

Needs to support complex math presentation and curation!

EXAMPLES

**CLASSICAL MOLECULAR DYNAMICS**

<b>PE</b>	<b>MR</b>
Newton's equation of motion	Lennard-Jones potential
$\frac{dV}{dr} = -m \frac{d^2 r}{dt^2}$	$V_{LJ} = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$

**FLUID DYNAMICS**

	Navier Stokes equation
<b>PE</b>	$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla \cdot p \mathbf{I} + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g}$
	Stress tensor for incompressible flows
<b>MR</b>	$\nabla \cdot \boldsymbol{\tau} = 2\mu \nabla \cdot \boldsymbol{\epsilon} = \mu \nabla \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T) = \mu \nabla^2 \mathbf{u}$



# The European Materials Modelling Council

MODA Portal: an online dissemination and data curation system



- Online interactive tool
  - Advanced **User interface**
  - A database backend
  - **searching**
  - **Metadata schema**
    - EMMO-schema encoded in Json, SQL and convertible to any other implementation, including HDF5 based
- Open development: <https://github.com/force-h2020/MODAPortal>
- Please check emmc.info soon for official test releases!



# The European Materials Modelling Council

MODA Portal: EMMC-Marketplace at: <http://emmc.info>



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SEARCH PAGES

SEARCH

SEARCH MEMBERS

Any field

Free text search

SEARCH

Participation  
Join the EMMC and contribute to discussions and activities

Blogs  
Read the latest blogs from translators, industry end users, ...

EMMC-Marketplace  
Find case studies and software tools and connect with peers!

Modelling Roadmaps  
Check the latest activities and engage in roadmapping

Document Your Modelling!  
Use the online tool to create and curate MODA

Networking  
See with whom we collaborate and network

Latest News

RECENT JOBS

Research Scientist in Computational materials engineering – material informatics  
Freiburg,

EMMC Brokerage and networking event 2017  
A specific session in the

Industrial Innovation Info Days 2017  
The European Commission is organising

EMMC Workshop on Interoperability in Materials Modelling  
7-8 November

EMMC Materials Modelling Workshop, Uppsala, Jun 2017  
15-16. June

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EVENTS

Interoperability in Materials Modelling

07/11/2017 - 08/11/2017

Cambridge

all events

SEARCH PAGES

SEARCH

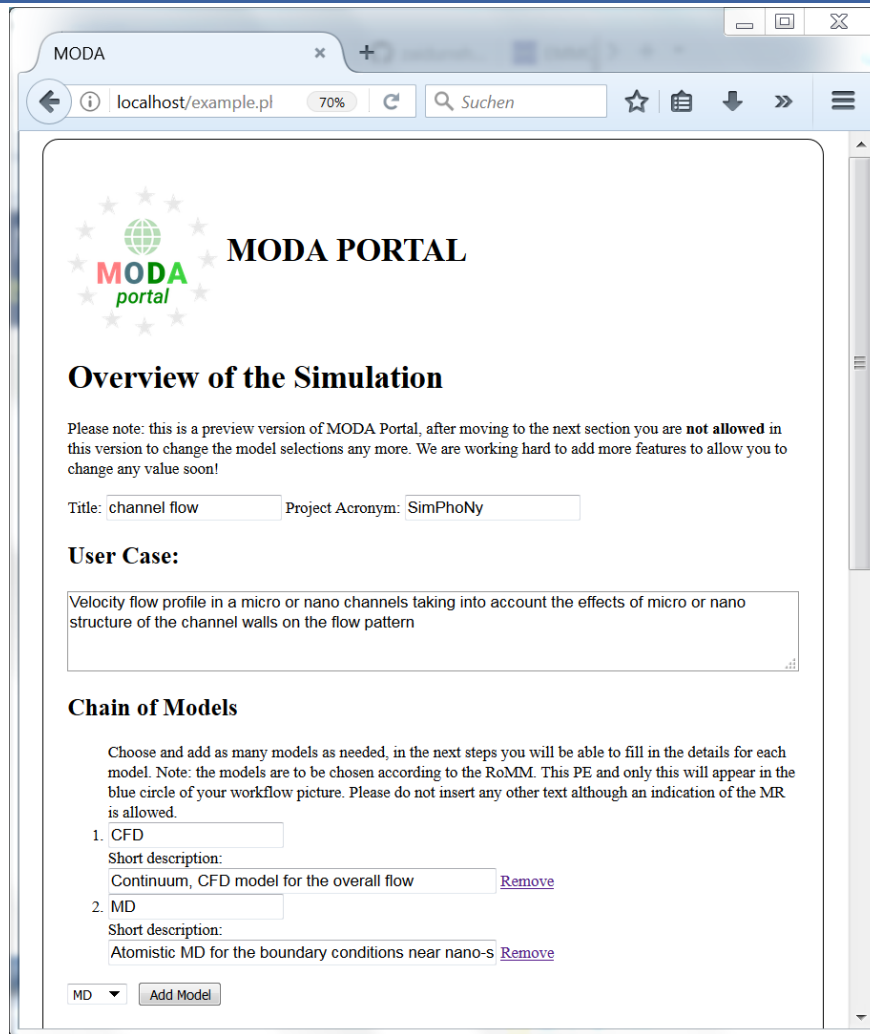
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MODA\_MOSTOPHOS 16\_08-2016

MODA\_ALLIANCE





The screenshot shows a web browser window with the URL localhost/example.pl. The page title is MODA PORTAL. The main content area features the MODA portal logo, a section titled "Overview of the Simulation", and a "Chain of Models" section. The "Overview of the Simulation" section includes a note about the preview version and a form with "Title: channel flow" and "Project Acronym: SimPhoNy". The "Chain of Models" section lists two models: 1. CFD (Continuum, CFD model for the overall flow) and 2. MD (Atomistic MD for the boundary conditions near nano-s). There is an "Add Model" button at the bottom.

Release preview after EMMC approval!  
(compliance to RoMM MODA)

Please contact me for an  
account for testing  
adham.hashibon@iwm.fraunhofer.de

- An EMMC MODA portal for managing materials modelling data presented in early preview. First public testing in September 2017!
  - MODA curation system
  - Integrated as a service of the EMMC-Marketplace initiative (see [emmc.info](http://emmc.info))
- **Accelerate exchange of information** between materials modelling codes and between modellers
- Integrated with EMMO-Schema putting data in a form that allows models and machines to **properly recognize** it along with its meaning.
- deal with the complexity of **sharing data between multiple tools** (in-house and commercial; proprietary and open)
- **Automatic code generation and workflow execution**



