Simulation Documentation With Materials Modelling Data Tables

European Materials Modeling Council (EMMC)
http://emmc.info

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The European Materials Modelling Council

The digital materials modelling marketplace

- 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 Welchy 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).

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

Why is MODA really good for you?

- 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.

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!

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EMMC plans for the **(very)** near future

- **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

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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!

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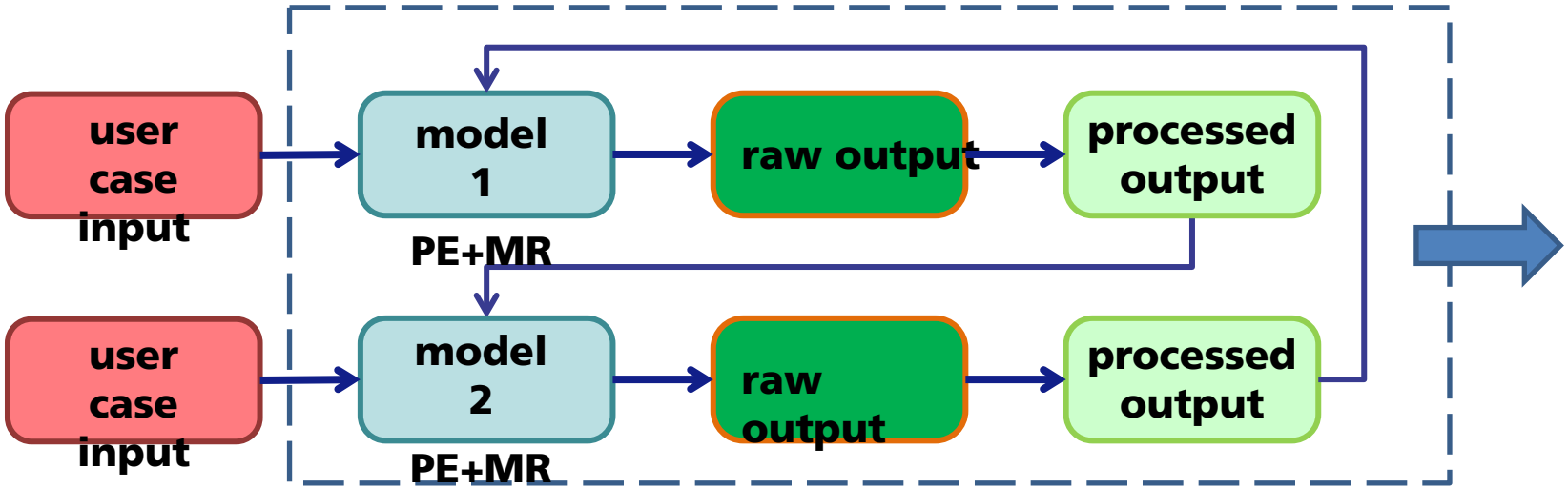
MODA Portal needs to support Workflow generation and curation

workflow for an iterative chain

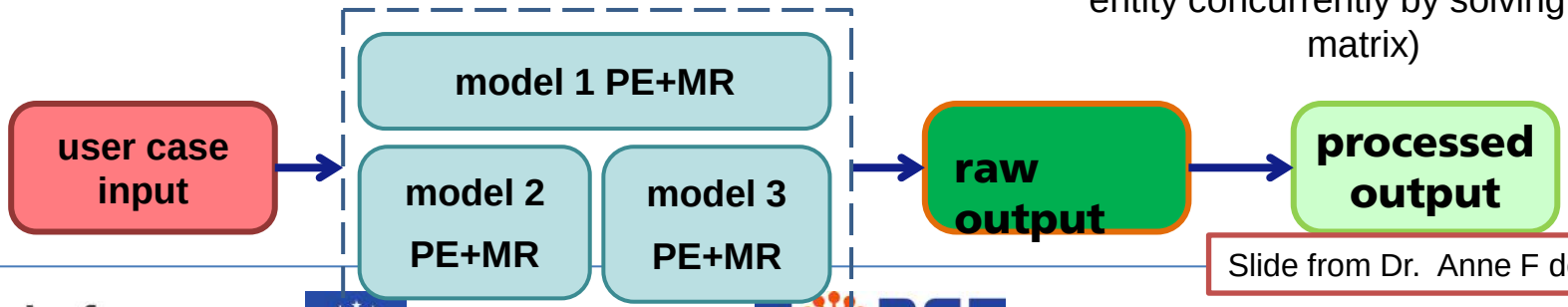
Iterative solution of segregated equations



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

MODA – Physics-based Model Definition

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

PE
Newton's equation of motion

$$\frac{dV}{dr} = -m\frac{d^2r}{dt^2}$$

MR
Lennard-Jones potential

$$V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

FLUID DYNAMICS

PE
Navier Stokes equation

$$\frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) = -\nabla\cdot p\mathbf{I} + \nabla\cdot\boldsymbol{\tau} + \rho\mathbf{g}$$

MR
Stress tensor for incompressible flows

$$\nabla\cdot\boldsymbol{\tau} = 2\mu\nabla\cdot\boldsymbol{\varepsilon} = \mu\nabla\cdot\left(\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}\right) = \mu\nabla^2\mathbf{u}$$

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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!

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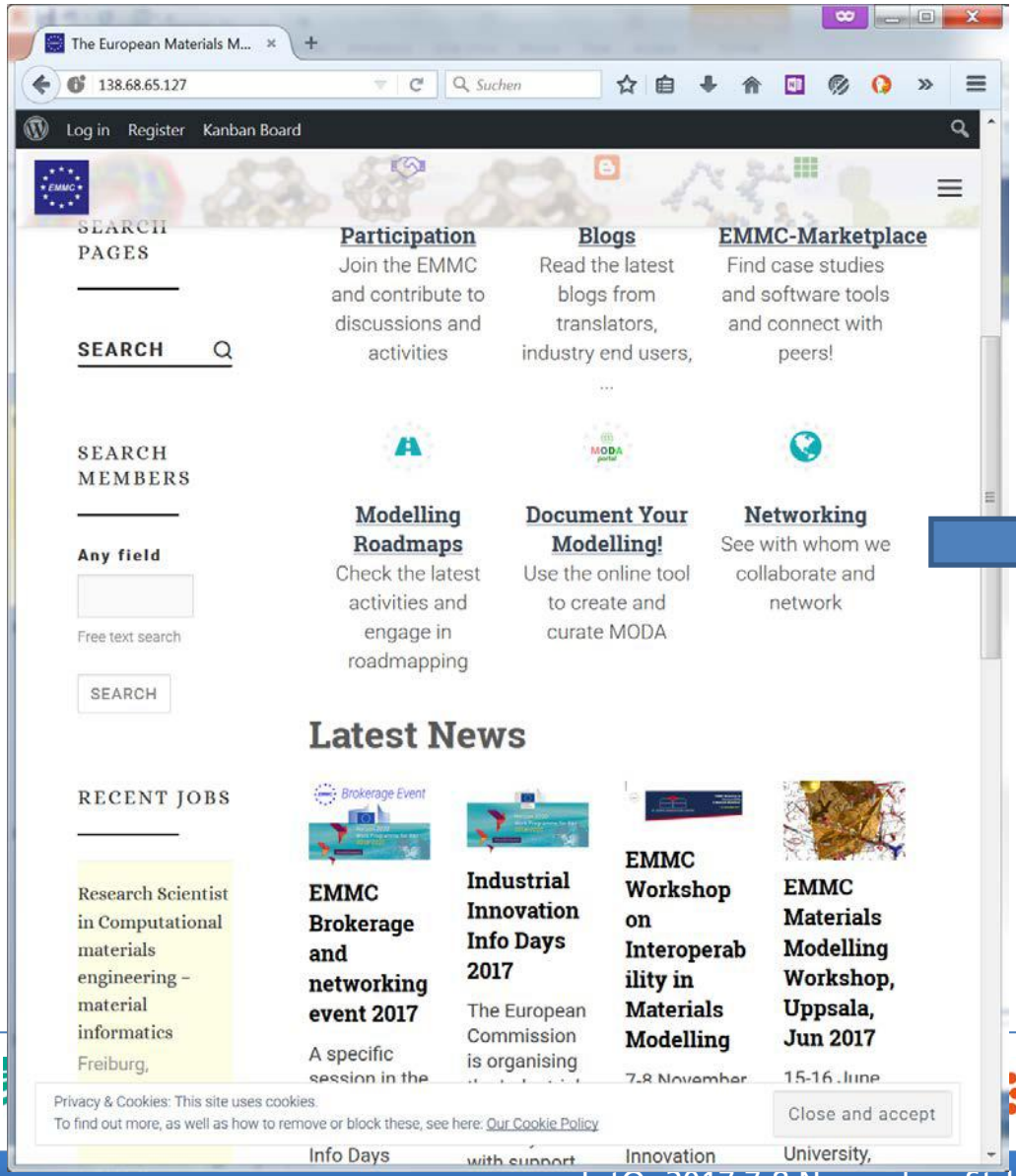
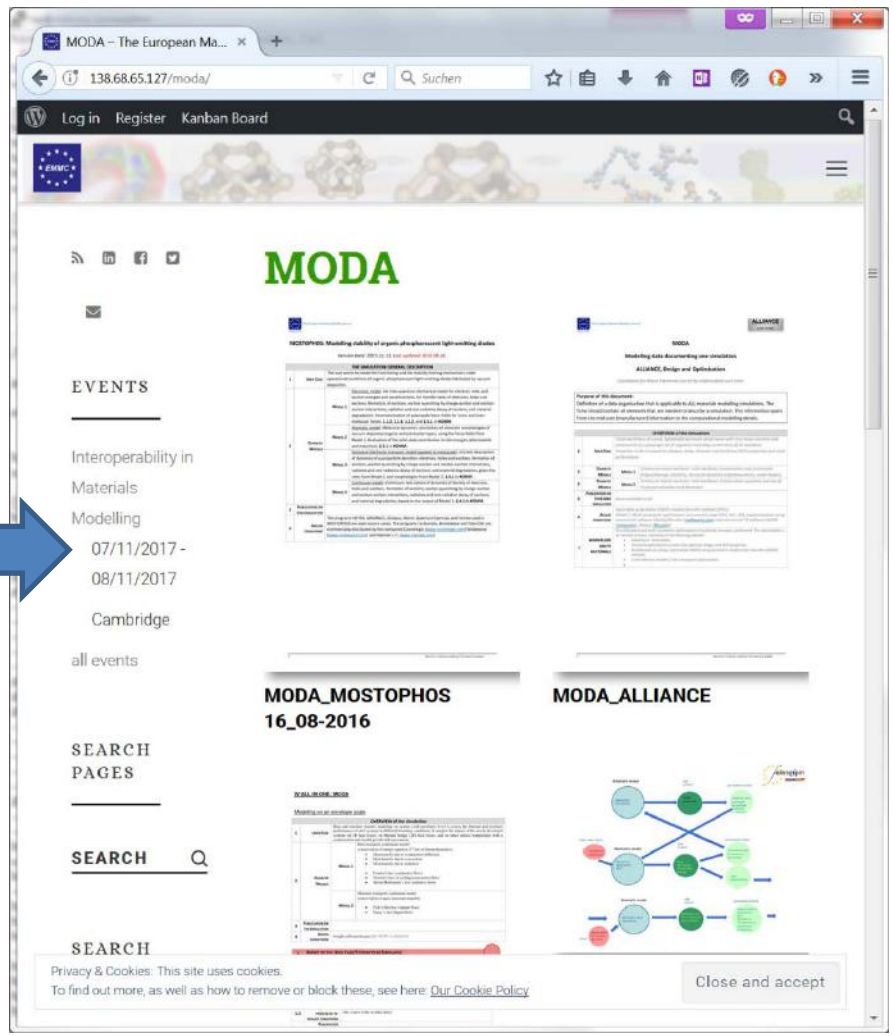
MODA Portal: EMMC-Marketplace at: http://emmc.info





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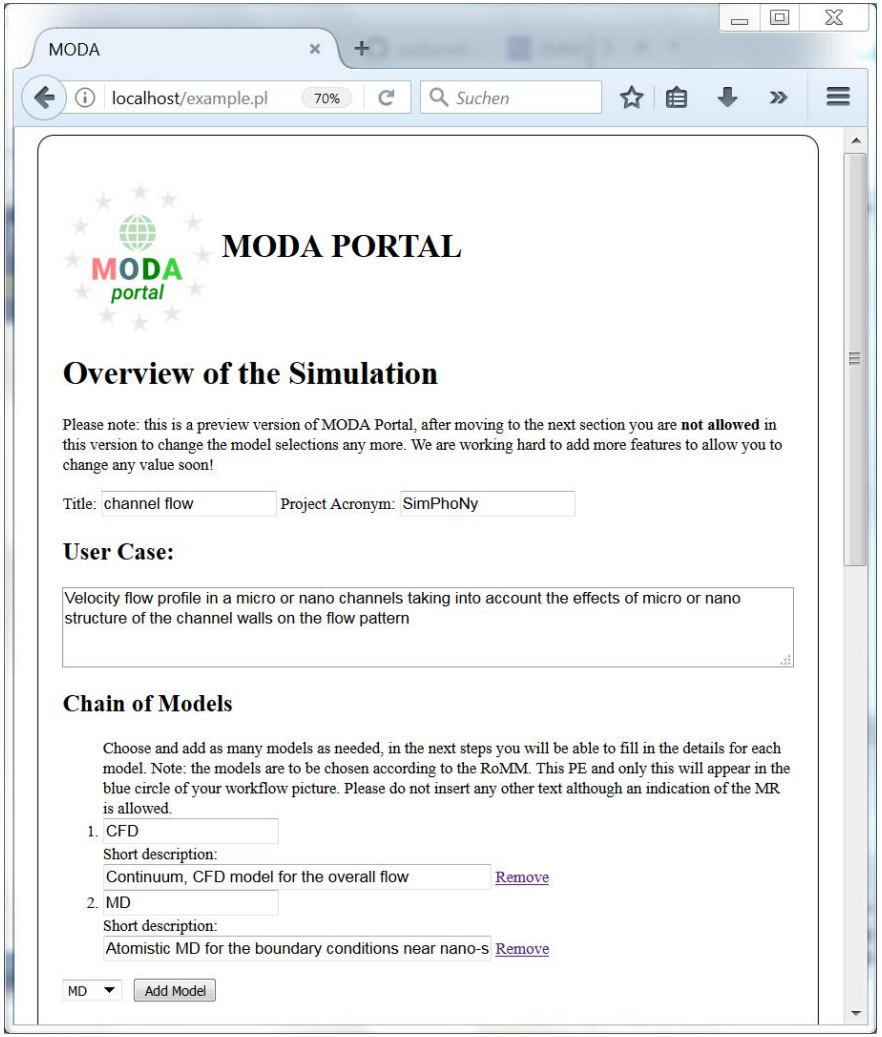
Quick Demo!



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

Please contact me for an
account for testing
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Summary and Outlook

- 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)
- **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**

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