Model development (electronic, atomistic, mesoscopic, ~~continuum~~, coupling & linking, ~~interoperability, open simulation platform, HPC~~):

Towards the Road Map 2017

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Road Map 2017 ?!?

The EC receives comments / feedbacks by stakeholders in the form of road maps.

- Road Map Feb 2015 (main focus of the current meeting) recommends topics/calls for 2016-2017, where the emphasis is not much on novel model development, but on exploiting the potential of existing models in industrial applications.

- **Road Map 2017** (November?) will address the calls in 2018-2019, where there will be room for model development towards industrial problems. Industrial endorsement is essential.

However the EC always listens...

Start working soon!

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Discrete Models (Electronic, Atomistic, Mesoscopic, C/L)

Some working groups (WGs) have already started to coordinate each other towards the Road Map 2017.

In particular, Electronic, Atomistic, Mesoscopic and Coupling & Linking (C/L) Working Groups have decided to merge and to promote actions under a common framework, called **Discrete Models WG**. The news will be visible on the public website of EMMC (www.emmc.info), soon after the meeting (with Charter, OTM and Deputy OTM).

Discrete Models WG, proposed structure:

- Electronic Models sub-WG
- Atomistic Models sub-WG
- Mesoscopic Models sub-WG
- Coupling/Linking sub-WG

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Discrete Models WG: Why merging?

Merge the “E+A+M+C/L" working groups into one discrete models WG.

- A merge has several advantages, namely → a stronger voice towards **overcoming difficulties in penetrating industrial practices** at large, a stronger voice in the discussion with other stakeholders in the EMMC. Moreover, many "discrete-model" modelers *de facto* already belong to several of the E+A+M+C/L communities. The discrete models have **many issues in common** (e.g. tuning the proper interaction potentials among discrete entities) and are naturally linked with and via Coupling & Linking WG.

Why not Continuum Models WG? Even though the Continuum Models WG is a natural partner for discussions and fruitful collaboration, continuum models represent already a well established practice in many industrial contexts. Hence promoting discrete models requires that we highlight their **special strengths**.

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Action Plan of the Discrete Models WG

The Discrete Models WG has already started to define an **action plan** towards the Road Map 2017.

The proposed Action Plan has been published on the wiki and it is open for discussion.

Action Plan for model development

Action plan for the discrete models WG (e+a+m+C/L) for 2015-2016

version: 12 January 2015; KH, PA, RC

Discussion page: Talk:Action Plan for model development, or simply press the discussion button above.

Action Plan
• Merge the "C/L+e+a+m" working groups into one discrete models WG (for reasons of clarity, strength and cooperation). • Drive an inventory of industrial "model needs". • Prepare for future call texts. • Actively drive strategic discussions about the role of models and model development inside and outside the EMMC. • Actively cooperate with other EMMC WGs and contribute to their strategic programmes (in a mutual fashion of course)

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Discrete Models WG: Inventory of model needs

Inventory of model needs endorsed by industry.

- Create an **application/industry-driven model/method-development wish list**, with the ultimate purpose to create industry-endorsed input for call texts for future H2020 calls. The **inventory** will also constitute a basis for the models part of the 2017 Road Map. We aim to have a first version of such a concrete list of most-needed models/methods and their entailing application contexts ready for publication on the EMMC wiki by the end of May 2015. Thus during February-May 2015, we need to contact various **industrial stakeholders** covering a range of important application areas, e.g. from the combined lists from EMMC events and from other contacts and channels. Then this list of topics will be further processed during the year. Input from Psi-k, CECAM, EUMAT, etc. will also be sought. Assistance and input from the WG members will be highly appreciated.

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Discrete Models WG: Complementary wish list

Model needs beyond already existing solutions.

- EMMC is currently in the process of collecting information about successful case studies, i.e. already existing solutions. The wish list/inventory of needed model improvements will in a sense be complementary. It should build on (i) experience gathered from modelling efforts where, despite being of current state-of-the-art quality, **the model limitations turned out to be an obstacle**, and of course (ii) modelling efforts which have not yet happened because they are still perceived as **unfeasible due to the lack of proper models**. Such a "negative list" will hopefully be a direct and important basis for the wish list and the upcoming call texts, and the success list will hopefully show that in certain fields materials modelling is already mature enough to make a real difference to industrial stakeholders [KH].

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Discrete Models WG: Not only dreams...

Discrete models represent already a **viable and effective tool** in many industrial applications.

- [Electronic] The prediction (Butler group, AL, USA) using electronic structure calculations of a large tunnelling magneto-resistance across MgO was later demonstrated experimentally and now in use in all read sensors incorporated in hard drives [RK].
- [Atomistic] Atomistic computer simulations of macromolecular receptors and their associated small-molecule ligands can play a big role in drug discovery, including the identification of cryptic or allosteric binding sites, the enhancement of traditional virtual-screening methodologies, and the direct prediction of small-molecule binding energies [Durrant & McCammon, 2011].
- [Mesoscopic] Coarse-grained simulations can allow one to design nanofluids, i.e. colloidal suspensions of nanoparticles, with desired physico-chemical and transport properties.

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Discrete Models WG: Setting the targets

The target audience of this inventory must be defined first. We aim to address people in **R&D departments** of the relevant industries, beyond **modelling experts** and practitioners.

It is important to prepare in advance a **guide** for the inventory. This could be a fixed list of questions, pre-defined options and categories, best practices, etc. This is essential for making easier the analysis of the inventory and for **post-processing the data**.

Example: The EMMC follows the categorization reported in the Review of Materials Modelling (EC). This categorization is **model based**, while the industry thinks **application wise**. Translation is necessary to identify the exact modeling content!

Some visual **litmus test** could be useful!

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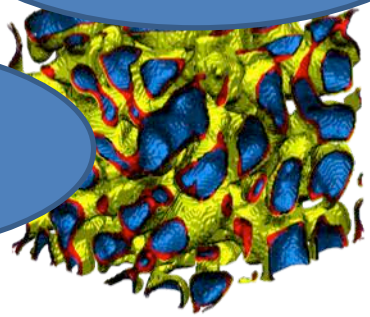
Litmus Test: Pick your own equations/entities first !!!

Equations and entities matter !!!

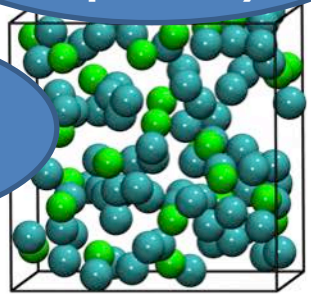
Conservation equations



Continuous Model

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0$$

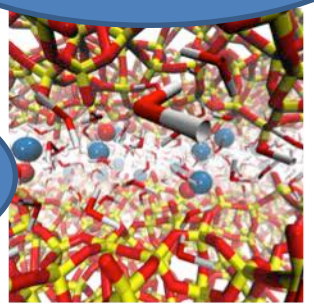
Diverse (e.g. Langevin equation)



Coarse Graining Methods

$$\langle \eta_i(t)\, \eta_j(t') \rangle = 2\lambda k_B T \delta_{i,j} \delta(t - t'),$$

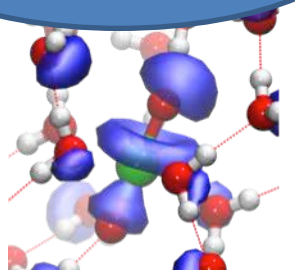
Newton equation



Molecular Dynamics Simulations

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

Schrödinger equation



Ab initio calculations

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left[\frac{-\hbar^2}{2\mu} \nabla^2 + V(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t)$$

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Discrete Models WG: Predictive modelling

Drive strategic modelling discussions.

- The models and the modelling methods constitute a crucial link in the modelling value chain and should have a central role in the EMMC. Members of the discrete models working group(s) are very familiar with the complexity and **difficulty entailed in the concept "predictive modelling"**, and the considerable obstacles that need to be overcome to reach there; this needs to be articulated in a strategic fashion. The EMMC, and the discrete models WG, should thus take an active part in, and help drive, this strategic discussion, in synergy with the other strong modelling organizations such as Psi-k, CECAM, and EUMAT.

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Discrete Models WG: Open effort

Enhance the Discrete Models WG's interactions with other groups and stakeholders of the EMMC.

- This concerns particularly the **Industrial Advisory Committee**, the **Continuum models WG** (clearly very important to us), the **Translator WG** (for obvious reasons), the **Software Owners WG**, the **Validation WG** (in fact we should jointly promote quality issues), the **MMP WG** (Materials Model Marketplace WG; which relies on the generation of good-quality data from good-quality models), the **Open Simulation Platform WG** (who should implement the C/L recipes). Clearly, the responsibility to achieve such fruitful interactions is mutual.

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Conclusions and perspectives

- Even though Road Map 2017 seems quite far away, it is an **important opportunity** to influence the model development in Europe.

- Hence proper strategic actions must be planned, taking into account the industrial practice, the value chains, **how modelling currently fits in the industrial value chains** and which opportunities are still there for novel models.

- An **inventory of model needs** (wish list) is considered an essential starting point. However it must be properly designed, both in terms of expected target stakeholders and guiding/auxiliary tools, in order to be really effective. Otherwise post-processing (unclear) results may become more demanding than performing the inventory itself.

Conclusions and perspectives

Thank you for your attention !!!

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Interoperability WG

The EMMC is starting a new WG on "**Software Interoperability and Communication Standards**".

- This group should deal with "Interoperability of software" and should co-ordinate all interested parties who want to be involved in the establishment of **communication standards** (a general and open language with a nomenclature for the necessary metadata). The interoperability workgroup should collect all actors in the field and become a strategy group, who builds an overview of all existing European activities in the field of software interoperability and communication standards and who gives direction to complementary activities.
- Communication Standards
  - Generic and structured list of **metadata keywords** and an **Alias Table** for keywords describing the same metadata.
  - Overall data structure for file based information exchange.

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Interoperability WG: NMP Projects Cluster

The EMMC Interoperability Work Group can rely on the **NMP Projects Cluster**.

- Five Collaborative Projects (DEEPEN, MMP, MODENA, NANOSIM and SIMPHONY) work on the definition of **software interfaces**, and the development of inter-process, and **inter-scale communication**. The project ICMEg (Integrated Computational Materials Engineering expert group) is a networking project (CSA) aiming to facilitate and develop an open and easily accessible formulation of a **global standard** for information exchange in ICME. A description of muti-scale modelling activities in several of the projects is appended.
- The 5+1 projects have agreed to cooperate in a **cluster** to work out proposals for meta-data and data structures for file based information exchange. The communications standards will be based on existing standards to the largest possible extend.

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Open Simulation Platform WG

The EMMC recommends to the EC to support the development of an open simulation platform based on the above standards which could be used to link and couple all existing materials models, as follows;

- Open Simulation Platform
  - Workflow tool(s) **to orchestrate a number of different materials modelling tools** (see Review of Materials Modelling for the scope of these tools); on one computer; first for linking than for coupling of simulations.
  - Tools for **distributed simulations**.
  - **Accounting schemes** (not for the use of the platform but for the use of commercial codes used in the platform operation by the user e.g. SME).