# REVIEW OF THE ROADMAP INCLUDING UPDATES & STATUS OF COLLECTED NEEDS IN EUROPE: KEY TOPICS NEEDING ACTION

*Coordinating Network*

*Integration of Materials Modelling in Business Processes*

*Modelling Market Place (data and code repository, expertise matching,..)*

*Validation of Materials Models*

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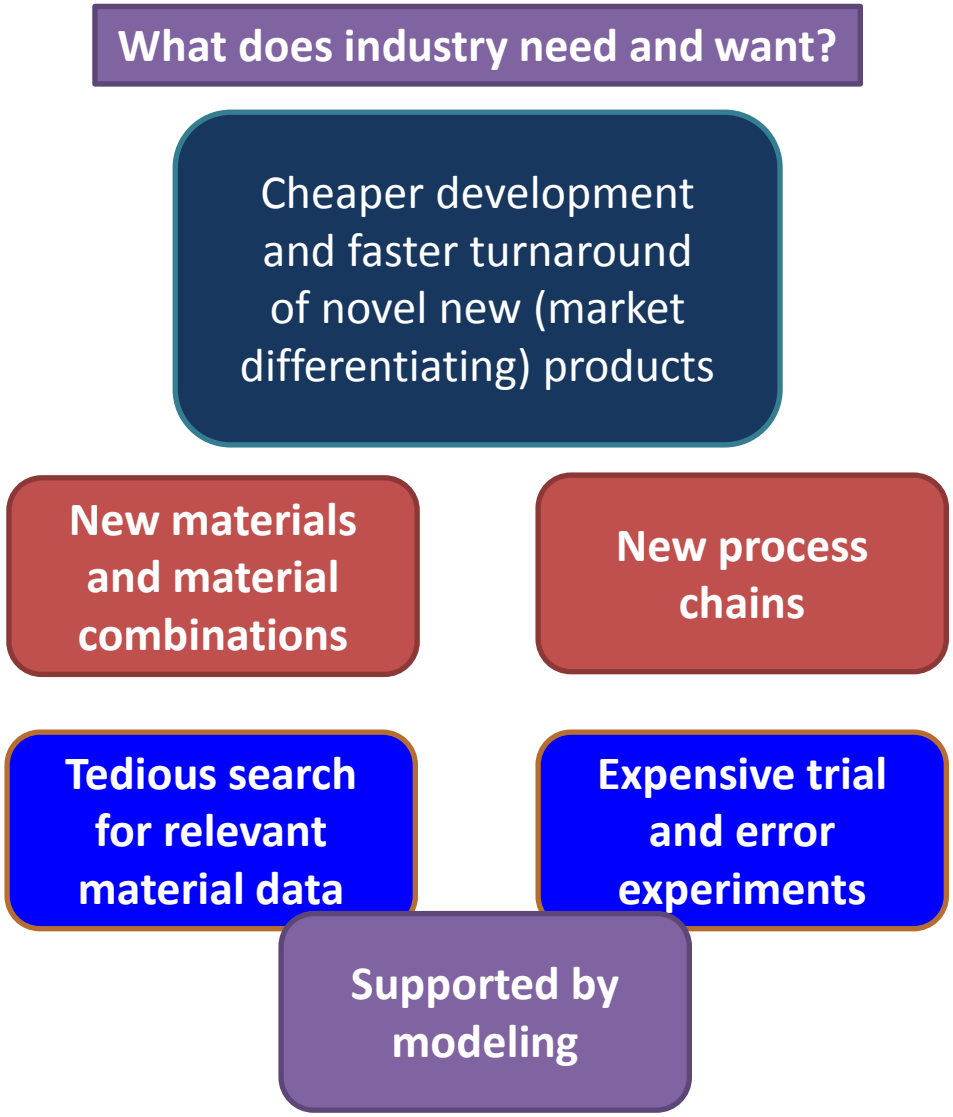
# The Big Picture: Where Are We Today?



# The Big Picture: Where do We Want to Go?

**What does industry need and want?**

Cheaper development and faster turnaround of novel new (market differentiating) products

**New materials and material combinations**

**New process chains**

**Efficient access to all relevant material data**

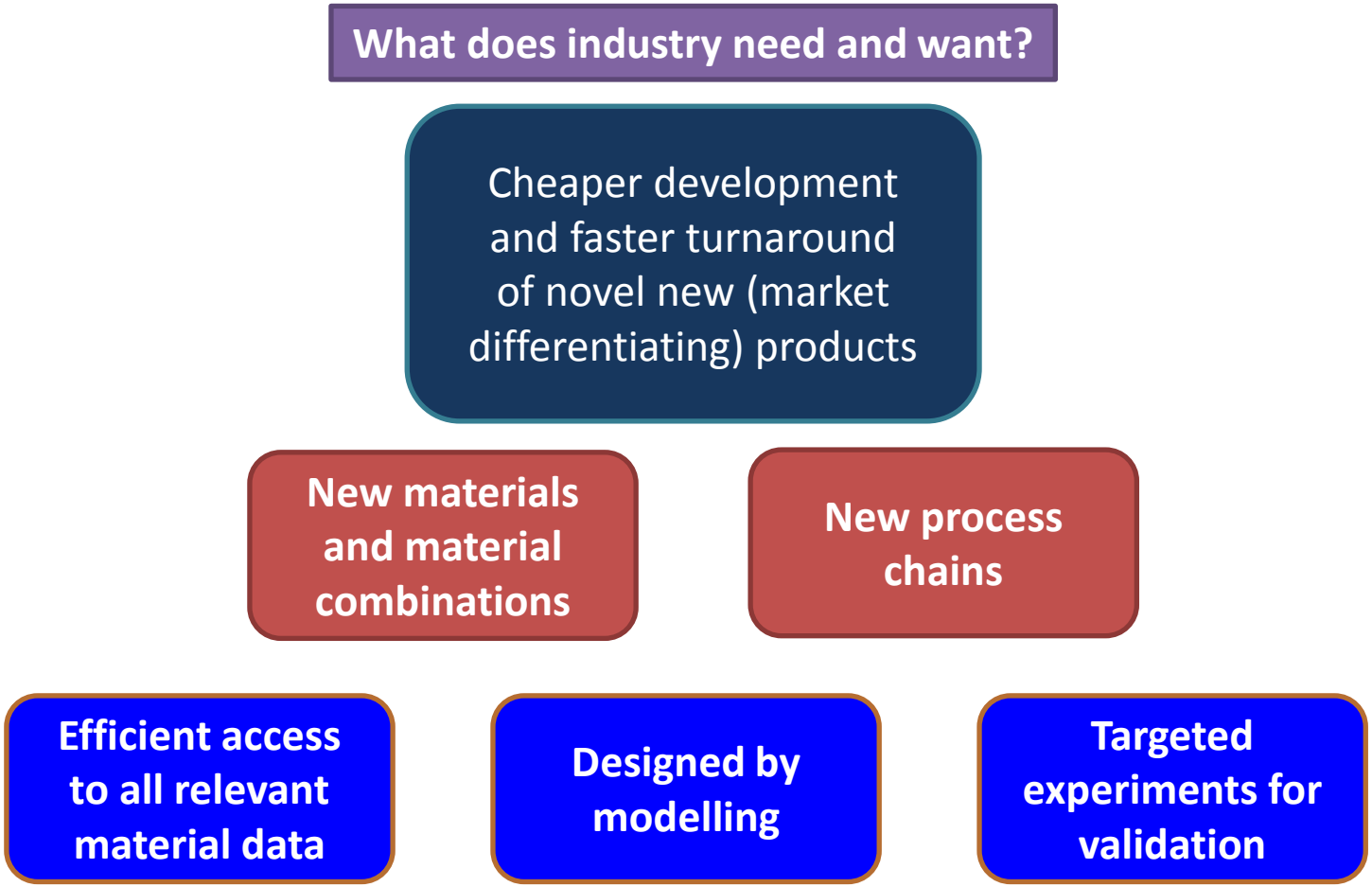
**Tedious search for relevant material data**

**Expensive trial and error experiments**

**Targeted experiments for validation**

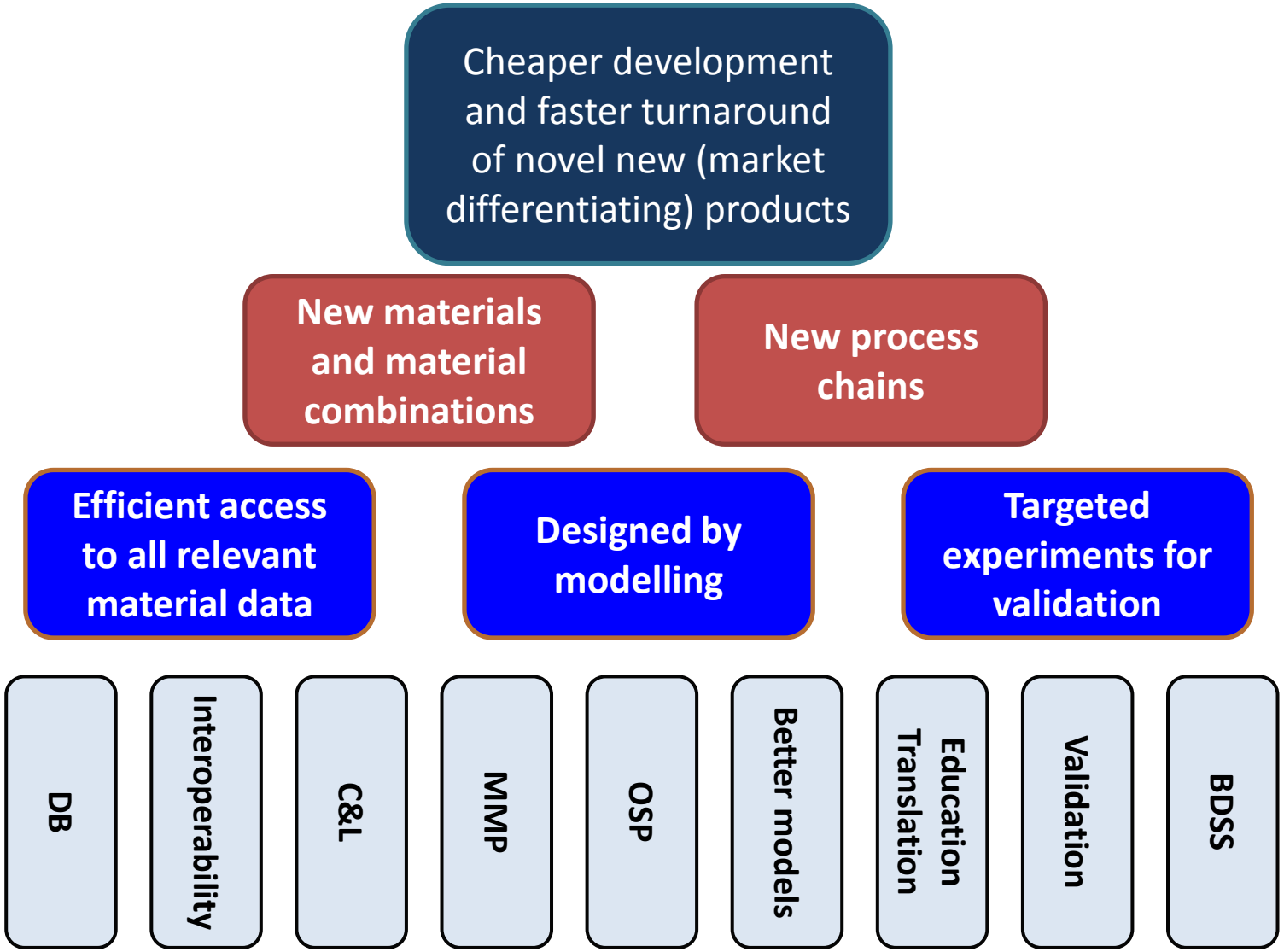
**Designed by modelling**

# The Big Picture: The Vision




Ultimate goal is to enable manufacturers to utilise modelling in their business decision support cycle, much as this is done today with experiments

# The Big Picture: How to Get There?



# What is the scope of the RM?

- The RM presents the needs of a large set of players in the materials modelling field
- The EMMC requests the EC to recognize the topics identified in the RM as topics of Europe-wide interest
- The activities proposed need to be developed to TRL7
- The implementation (TRL 8-9) will be up to the individual organisation/academic or company and can become a proprietary exercise
- Input ontained from the entire
- The EMMC strives to identify gaps and actions to address them based on a rich input from and discussion between **all modelling communities** (MAN, TRANS, SWO, MOD) in the EMMC

# Focus of the Current RM

- The wide European stakeholder consultations conducted within EMMC proposes that the EU-LEIT **Work Programme 2016-2017** should be used to:
  - Exploit the materials models that exist
  - Focus on successful transfer to the industry to capitalise on the enormous potential
  - To support this with:
    - Coordinating networks
    - Integration with business processes
    - A modelling market place
    - Validation tools (databases and interpretation tools)

# 1st draft of the Roadmap for Materials Modelling

- Active discussions were conducted during the EMMC-KoM across four different sessions representing all stakeholders
- The discussions were summarised and documented in discussion minutes
- The minutes + discussion notes of the EMMC WGs resulted in the first draft of the Materials Modelling RoadMap composed by all session leaders

- The draft of the RM was published on the EMMC website and wiki (22.12.2014)
- EMMC members were invited to give feedback on the wiki
- Feedback was open also to non EMMC members (by registering first to the EMMC)

# 2nd draft of the Roadmap for Materials Modelling

**Step 1. Collecting feedback and updating the RM:**

- Feedback was very lively, productive and helpful in shaping a new updated and more refined RM document
- All feedback topics where carefully analysed
  - Are the topics already covered in the RM?
  - Do they reflect some lack of clarity in the RM?
  - Are they completely new points?
  - Do they fit into the RM (i.e., in the scope of the LEIT program)?
- Update process:
  - We tried our best to convey all points into the new draft
  - Over 400 revisions in draft 2
- **Step 2. In today's meeting, discuss and finalize the RM**

# Summary of Feedback from the wiki

| Thread title | Replies |
|---|---|
| Business decision support system - Clarification | 0 |
| What do we need to model? | 17 |
| Some possible actions | 1 |
| Translation Process | 13 |
| Success Case | 6 |
| Materials Modelling Marketplace | 4 |
| Open Simulation Platforms | 6 |
| Exploit better the existing industrial value chain | 10 |
| priorities of EMMC | 0 |
| Model as the core knowledge | 1 |
| Business Decision Support Systems | 1 |
| Where we are today - Chapter 3? | 1 |
| Origin of materials data for FEM models | 1 |

- 61 discussions, 13 topics (threads)

# Summary of Main Revisions

- BDSS section almost rewritten, role of BDSS clarified
- Big-data analytics and artificial intelligence in MMP, Databases and BDSS
- Translators definition as new players is more precisely defined
- Case studies and approaches that do NOT work are recognized in Validation, BDSS, MMP, and Databases,
  - also as a driver for new model needs and developments
- Synergies between MMP-BDSS-TRANS was made more specific and clarified
- IP issues, data sharing policies and openness in the MMP was addressed more specifically
- Differentiation of OSP from existing commercial software tool chains is addressed and clarified
- More details on the advantages of standards and interoperability
- New input on Software Guidance and exploitation (as an appendix)
- Process recipes are recognized in the RM as having strong effect on the characterization of materials
- Specific reference of TRL levels in publicly funded projects
- emphasize the positive synergy between market and research (i.e., where public projects stop and commercial exploitation starts)

# This is Just the first step!

- This Roadmap addresses many of the challenges
- More will surely come up
  - **The EMMC Road Map will be renewed and updated in the coming two years to generate the next EMMC Road Map by the end of 2017**

# INTRODUCING THE ROADMAP

# Where are we Today

- Today, modelling is not yet always the essential tool in commercial development
  - difficult to use
  - not accurate enough, not validated enough
  - cannot deliver specific answers to specific questions
  - not easy to integrate into closed loop optimizations
- The ultimate goal is that materials modelling and simulation **will become an integral part** of product life cycle management in European industry
  - This is dominated by continuum methods but smaller scales are important
- The EMMC aims to stimulate the industrial exploitation of discrete modelling approaches in industry by linking them to the already well-established continuum-models
- Coupling and linking and integration are key needs

# Key and Main Topics

- The RM addresses a number of key topics in details stating for each
  - Where do we want to go? How do we want to get there? and Actions
- Key and main topics:
  - Coordinating Network
  - Integration of Materials Modelling into Business Decision Support Systems
  - Translation
  - Modelling Marketplace (MMP)
  - Design of a System of Databases
  - Model Development (separate session)
  - Coordination of European developments on Interoperability of Software and Operational Simulation Platform
  - Validation of Material Models
  - Design of Case Studies
  - Stimulation of academic software exploitation

# Coordinating Network

- There is a need for a coordination network in materials modelling that can support
  - Integration of material modelling in business (BDSS) and industry
  - Development of the role of translators
  - Establishing road maps for model development
  - Coordination of existing activities on interoperability of software and operational simulation platform developments in Europe
  - Design of a system of databases, validation and interpretation tools
  - Design of case studies demonstrating the industrial potential
  - Stimulation of academic software exploitation and engagement of SWO
  - Development of modelling market place (MMP)
- The RM proposes a set of actions (CSA, IA, RIA) to achieve these goals
- We advice the EC to open a call for a CSA for coordinating network

# Integration of Materials Modelling into BDSS

**Where do we want to go?**

- Generic tools for the integration of material models with business criteria and "big-science & technology and business data"
- Allow technical and commercial decisions that minimize risk and maximize the success rate of actions
- Allows multi-objective optimisation combining materials models and experimental data to develop option scenarios and consequence analysis
- The BDSS intention is not a replacement of internal established commercial processes specific and confidential for each company

# Integration of Materials Modelling into BDSS

**How do we get there?**

- There is a need for the development and implementation of **methodologies** for **flexible integration** of material models and commercial decision process
- Need to define **standards** and a high level language/set of parameters that will constitute the backbone of the integration step.
  - These needs can be greatly assisted by the EMMC Modelling Marketplace (MMP) and Open Simulation Platform (OSP) activities.
  - Translators can then complete the cycle by using the MMP, OSP, and BDSS to connect to the end users

# Integration of Materials Modelling into BDSS

**Short Term Actions:**

- Develop case studies, where integration of different modelling levels have led to successful decisions
- Communicate "company inside" success stories to the right level stakeholders and decision makers (by using the EMMC-MMP)
- Collect feedback from end users (PR)

# Integration of Materials Modelling into BDSS

**Medium and long term Actions:**

- The EC can fund the development of the generic tool from TRL3-TRL7 leaving the customisation of the tool to commercial players and other end users
- Education in this holistic view is key and the EMMC encourages the EC to promote education towards this goal.
- RIA is recommended for the initial design of a generic BDSS: workflows, best practices in the medium term, followed by the development of a software platform for BDSS, interfaces to model software integration and convenient set up of KPI models; multi-valued optimisation problem solver and integration

# Integration of Materials Modelling into BDSS

**Discussion: <to be filled interactively>**

# Modelling Market Place

**Where do we want to get to? (part 1)**

- ***Vision:*** strongly connected communities of various stakeholders which have access to a Hub providing a vibrant digital **collaboration tool** with
- Databases (of data and knowledge)
- Provide a **model selector** for the right set of workflow components and a set of experimental data to validate the models in a new specific application (to be used also by BDSS and TRANS)
- **Big-data material informatics and analytics,** systematic data mining (e.g. by artificial intelligence, model reduction, quantitative structure/activity/-property relationships, etc.)
- I**nformation exchange** on best practice, validated methods and information about approaches that have been found to be unsuccessful, or insufficient, for certain cases.

# Modelling Market Place

**Where do we want to get to? (2)**

- Provide means to handle Intellectual property, ownership, and sharing policies
- Promote the sharing of data and a vibrant Eco-System
- Enable coupling/linking of all components in and effective, easy and maintainable way
- C&L models need to be developed and wrappers (interface software) are needed for models and databases to talk to each other and these can be developed based on the new standards
- Enable data quality to be tested against experimental data using automatic means (artificial intelligence).
- Provide additional publication and dissemination avenue

# Modelling Market Place

**How do we get there?**

- The MMP will require input and involvement from all types of stakeholders
- MMP development will rely on input and collaboration with manufacturers on IP issues and sharing policies
- BDSS and TRANS would deliver case studies and workflow use cases, as well as big-data analytics requirements
- MMP will develop the integration schemes, wrappers, and big data analytics (with machine learning, artificial intelligence, search, and metadata structuring, etc)
- Standards are needed for optimal information retrieval and interoperability of different components
- An operational simulation platform will assist by promoting the use of software wrappers that are needed for databases so they can talk to each other. The involvement of the SWO in this is desired.
- Translators would assist in identifying the intended audience of MMP

# Modelling Market Place

**Actions – short term**

- 1Q.2015: Initial survey of available database and content management systems and suitability to the MMP requirements
- 1Q.2015: initial requirements and USE CASES for the future MMP site (including databases of models, data and wrappers)
- 1Q.2015: Move the wiki-emmc.org and emmc.info into one home
- 2Q.2015: Publishing new form/questionnaire for the database of actors (DBA), to be linked with the wiki and emmc.info
- 3Q.2015: Publishing the first component of the MMP: DBA
- 2015 and beyond: assembling and coordinating existing activities related to the wrapper and databases requirements and operations within EMMC
- 1Q.2015 MMP will start investigating the IT behind existing databases and start designing a common interface (experiment on wiki-emmc.org and emmc.info)
- 3Q.2015: Meta-database of models (input, software descriptions, stakeholders)
- 4Q.2015: linking the model database to the DBA: first version of the marketplace

# Modelling Market Place

**Medium and long term actions (part 1)**

- CSA is needed for assembling and coordinating activities starting from 2016/2017.
- RIA projects or one big IA are needed to implement a set of standardised, clustered databases.
- In the CSA action:
  - Concentrate on assembling and coordinating existing activities related to the resources and databased of wrapper operations for simulations and databases.

# Modelling Market Place

**Discussion: <to be filled interactively>**

# Validation of Material Models

**Where do we want to get to**

- Industry requires validated material models to integrate into the BDSS
- Quality attributes need to be determined based on both accuracy of modelling and business requirements
- Need to coordinate the necessary characterisation and validation methodologies
- Experimental database curation is key for validation
- Quality of data must be continuously challenges to prevent stagnation
- High quality documentation is needed
- Use frequency of data and user feedback are needed to assure quality
- There is a need to structure raw data including procedures, and separate interpretation from primary data
- Modeling Market Place, BDSS, and Translation are essential ingredients

# Validation of Material Models

**How do we get there?**

- Metadata is key
  - Structuring (standardisation) of raw experimental data with workflows (protocols) needs to be investigated (MMP, BDSS)
  - CUDS should be extended to cover experimental data and workflows
    - Will enable ICME procedures
    - Enable integration into BDSS

**Actions**

- A CSA is recommended to design a validation infrastructure to enable:

1. Data handling, including data mining and linking data
2. Calculation of materials properties from the raw experimental data
3. Development of new test facilities/devices and experimental protocols adapted to the needs of validation.

- RIAs or one large IA is recommended to develop the content of a virtual EU platform of laboratories able to carry out experiments and validation of models.

# Validation of Material Models

**Discussion: <to be filled interactively>**

# Coordinating Network on Interoperability

**Where do we want to go**

- Interoperability of software is key to BDSS, TRANS, Databases and automated (closed-loop) optimization
- Future materials research will rather need modular software structures and not monolithic solutions
- Need to orchestrate the interplay of different software tools
- Efficiency requires standardized information exchange
- **Need to coordinate activities in EU to agree on standards**
  - Essential, otherwise EU SWO and MAN will be faced with de facto international standards that do not take into account the interests and needs of EU markets, undermining their competitiveness
- Standards must be open, and freely communicated to all stakeholders
- Focus on standardized file exchange

# Coordinating Network on Interoperability

**Where do we want to go**

- The EMMC thus requests the EC to recognize this European-wide interest and to fund an OSP and support its development from TRL3-7

- Software vendors can customize the result and commercialise it

- The EMMC believes this will strongly increase the exploitation of all existing software tools - academic and commercial in Europe. It is further believed that the combination of these tools in a platform structure will lead to new insights and to the development/qualification of new materials and new processes at a much higher pace.

# Coordinating Network on Interoperability

**How do we get there**

- Global coordination to avoid fragmentation and lagging behind international actions
- International efforts are ongoing within the ICME community
- Active participation of EU SWO for setting needs, requirements and acceptable standards is important

# Coordinating Network on Interoperability

**How do we get there: 10 year planning in the RM:**

1. developing the metadata standard (e.g., keyword bases) for models
2. creation of technical basis for Common Universal/Unified Data Structures: CUDS
3. publication of the CUDS specifications

- **Together with the Modelling Market Place we should**

4. assemble software tools covering all scales and stimulate the development of wrappers for them
5. assemble solvers used to solve the physics equations and ensure they can be integrated into the platform
6. assemble data processors like homogenisation tools including volume averaging etc. and ensure they can be integrated into the platform
7. assemble “estimator tools" and ensure they can be integrated into the platform
8. assemble wrappers
9. reflect on database technology

# Coordinating Network on Interoperability

**Actions**

- CSA is recommended to agree and promote communication standards (as a start, first at EU level) between EU software owners, manufacturers and modellers.
- RIA is recommended to design a new system that can integrate materials modelling components used in industry.
- It is advised to allocate efforts in EU-LEIT projects on the use of standards and actively contribution to their development.

# Coordinating Network on Interoperability

**Discussion: <to be filled interactively>**

# Design of a System of Databases

**Where do we want to get?**

- The overarching goal of the EMMC in this domain is to establish leadership in "sharing data across modelling fields
- The long term goal is to establish an exchange/interpreter of databases that for a specific material gives e.g. the electronic structure, atomic nuclei positions, particle/grain and continuum behaviour.
- Establish a holistic modelling approach and thus produce realistic predictions of materials behaviour under real world conditions.
- Key is to coordinate subfield activities so that available data become visible to all stakeholders in all subfields.

# Design of a System of Databases

**How do we get there?**

- Two databases are proposed, one for simulation data and one for experimental data
- **Reproducibility is key**
- Requirements and design of database with simulation data.
  - *Step 1: Database of simulations (metadata only: code and input)*
    The first step is a co-ordination of databases in subfields. Gathering information on already available data and making this visible to all stakeholders in all subfields is to be stimulated.
  - *Step 2: Gold Databases of simulations (input, code, raw output data)*
  - *Step 3: Database of Materials properties*
  - *Timeline: 2017 at the earliest*

# Design of a System of Databases

**How do we get there?**

- Requirements and design of a database with characterisation data (raw data)
  - *Step 1: Interface modellers-experimentalists*
    - a) Inventory of existing characterisation databases for interest for validation of models (database types and content)
    - b) Modellers define guidance for data needed for validation of their models
  - *Step 2: Elaboration of the characterisation database*
- An exchange methodology should be elaborated to interpret and share the information in the different subfields so that a structured exchange is generated and supported.
- Requirements and Design of Website facilitating beta testing of codes under development
- *Timeline: earliest 2018-2019*
- Design of tools for interpretations of raw characterisation data
- Requirements and Design of tools for validation of constitutive equations
- Case studies with examples on how these databases function for dissemination

# Design of a System of Databases

**Actions**

- The development of the databases is proposed to be part of the CSA on networking for the initial design and to be part of RIAs or an IA for the new modelling market place.
- The CSA should take on the role to actively stimulate the filling of the database.

# Design of a System of Databases

**Discussion: <to be filled interactively>**

# Translation

**Where do we want to go:**

- Industry needs neutral players that translate industrial problems into cases to be simulated
- Translation is a role to be stimulated, SWO, R&D departments but also special actors can take up this role
- Aim at creating a set of open and transparent conditions and best practices as well as a resource of neutral competences available to all industry more widely, in particular to SMEs
- The new Translator role significantly supports and enhance the role of R&D in companies
- Develop Key Performance Indicators (KPI) that include also and relation to business related measures like pricing and time to solution, etc.

# Translation

**How do we get there?**

- Develop a code of conduct, NDA
- Document industrial success stories of translation efforts
- Identify best/worst practice communalities, set up a best practice guide for translation
- Develop draft of a methodology for the analysis of industrial problems
- Translation experiments: use Translators methodology in order to identify necessary improvements on the Translators methodology

# Translation

**Actions**

- A CSA is recommended to develop the role and functioning of translators.

# Translation

**Discussion: <to be filled interactively>**

# Model Development

**Where do we want to get?**

- **See dedicated session (Pietro Asinari)**
- *Better, more accurate, reliable and efficient models and methods*
- Predictive modeling
- Taxonomy of models and capabilities (related to the Modeling Market Place)
- Needed workflow
  - Models and model development: leads to database of models and simulation data
  - Coupling and Linking of models: leads to new multiscale science, enable to model phenomena that cannot be described by one scale alone
  - Validation: to deliver information on the applicability and accuracy of modelling (and in some cases augment modelling data with experimental sources)
  - Integration of models (using the OSP) and databases infrastructure (MMP/DB): enable the modelling of device and process level systems.
- **See also separate session by Pietro Asinari: *Model development***

# Model Development

**How to get there?**

- calls or actions targeted at “widening models” as opposed to extending simulation methods are needed.

**Actions**

A CSA is recommended to set up a Road Map with an analysis of necessary material model development for specific problems relevant to industry need to be conducted. Existing mesoscopic modelling approaches should be categorised according to the most relevant features, namely the granular description, and those models without should be excluded. The Road Map should also include novel coupling and linking methods. The analysis should be conducted across the board.

# Design of Case Studies

**Where do we want to get?**

- Case Studies are important to convey the benefits of material modeling to industry
- Use Cases are vital for extracting and defining specifications and requirements for:
  - user interfaces and key algorithmic and development specifications of databases, Validation, MMP, BDSS, and
  - Determine priorities for feature Integration (of modeling)
- Strategic coverage of Industrial demands should be ensured by the set of case studies
- Case studies should cover both success stories, and cases where lack exists
  - Igniting therefore targeted development of models and methodologies
- Keywords to classify case studies categories should be agreed
  1. Use of materials models and databases in an industrial environment
  2. KPI models, benchmark problems

# Design of Case Studies

**How we get there?**

- Translators may be able to identify Use Cases of modelling software tools including databases based on their experience with industry.

**Actions**

- An initial set of case studies will be created by the EMMC based on input from the Manufacturers stakeholder group.
- A conference could be organized by EMMC focusing specifically on how to replace test setup and mock-ups by numerical simulation.
- A CSA is proposed to collect and elaborate further case studies, including success as well as failure examples

**See also separate session by Gerhard Goldbeck: Identifying Case Studies**

# Stimulating Academic Software Exploitation

**Where do we want to go?**

- More efficient transfer of academic software to industry
- Need better codes, data standards and integration of codes (clean API, open standard data specifications).
- Three phases have been identified by SWO:
  - Phase I: Exploratory Phase (fundamental science)
  - Phase II: new material modelling software (non commercial, TRL 3-7)
  - Phase III: Commercial (TRL > 7), LTS, documentation, verification
- Target of EU-LEIT is Phase II, bridging the “gap over the valley of death”
- SWO can take this to Phase III
- Should happen with original academics that wish to be part of the exploitation, possibly in collaboration with Translators

- **See also separate session by Erich Wimmer: *Recommendations for academic materials modelling software engineering***

# Stimulating Academic Software Exploitation

**Where do we want to go?**

- To ensure continuity: standards and openness leading to better maintainability, and quality are needed
- Academy should adapt software engineering paradigms (better code, testing, verification, documented test cases, etc)
- SWO have genuine interest in participating in EU programs to provide close guidance on software engineering from the start of development
- Licensing schemes must allow exploitation later
- Academic partners should have a fair chance to participate in the exploitation process (harvesting the fruits of their work) along with translators
- Data standards can also lead to lowering the cost and efforts for transferring software to commercial exploitation later

# Stimulating Academic Software Exploitation

**How do we get there?**

- Guidelines for good software engineering should be formulated
- Workshops for software engineering are needed
- Stronger emphasis on the application of best practices, standards (both for data and API when possible) in publicly funded projects

**Actions**

- SWO to organize a white paper on software quality and software engineering advice.
- TRL's specifically designed for software development should be developed based on the H2020 TRLs
- The EMMC should make an inventory of the training on software engineering available.
- The EMMC should agree a whitepaper on licencing recommendations agreed with all stakeholders
- The EMMC should elaborate communication actions towards academic developers concerning drawbacks and pitfalls of different licensing schemes.