



# The European Materials Modelling Council

## *Project idea presentation template*

- You can use a free template, but please keep EMMC logo above.
- Maximum 5 slides (approximately 3-5 minutes for presentation).
- Outline of the presentation (mandatory contents):
  1. What is the call/topic number? e.g. NMBP-09-2018
  2. Who is the main contact? Provide contact details
  3. What is the name and the subject of the Project idea?
  4. What are the main objectives of the Project?
  5. What are the innovative aspects of the project idea?
  6. What are the expected results? Refer to TRL
  7. What is the expected impact?
  8. Is there any demo building available already identified?
  9. Who are the identified and the missing partners?

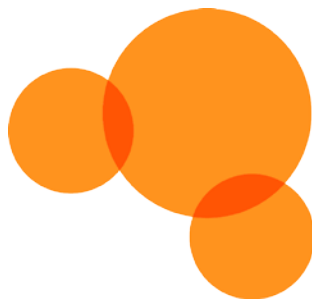


# The European Materials Modelling Council

## *Project idea presentation*

Call topic: [DT-NMBP-09-2018](#), *Accelerating the uptake of materials modelling software*

Main contact:



# SCM

Software for  
Chemistry &  
Materials

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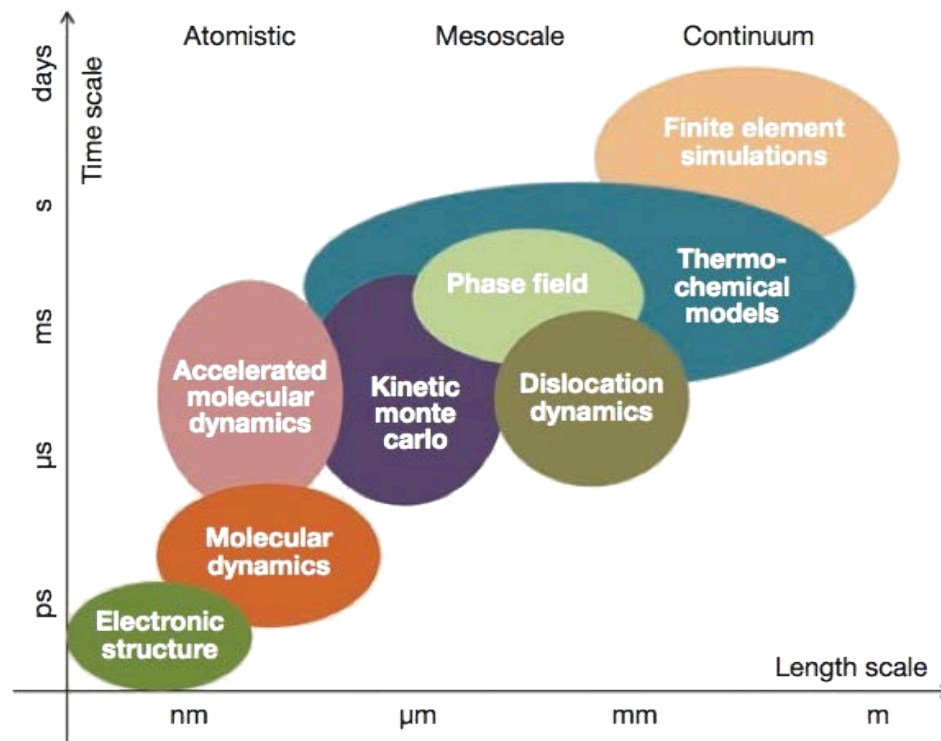
Project name: *Multiscale Computational Framework, from Molecules to the Continuum*



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## *Project idea presentation*

A project bringing together experts in commercial and academic software development to couple scales from the molecular to the continuum, integrating existing tools into a user-friendly multiscale modelling platform that will be validated and demonstrated in pilot-scale and industrial case studies.





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### Main objectives:

- To **integrate discrete and continuum** modelling approaches from the electronic to the continuum scale into a seamless modelling framework.
- To facilitate **faster product development** thanks to a **user-friendly** software platform.
- To build on current **standards for semantic interoperability** across domains.
- To **validate** the platform via case studies motivated by stakeholders' needs.
- To make the platform **available via an online marketplace**.

### Innovative aspects

- Focus on the **usability of existing codes**, to facilitate use by non-experts.
- Exploration of **marketplace-based business models and exploitation plans** for European academics, RTOs and SMEs.
- Emphasis on **extendability and interoperability** with other codes.



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### Expected results:

- Multiscale modeling framework integrating academic and commercial codes (currently validated in lab, TRL4).
- Integration with existing and emerging EMMC marketplace(s).
- Marketplace-based business models and exploitation plans.
- Prototype demonstrated in operational environment, with industrial partners (TRL7)

### Expected impact:

- Increased innovation in industry based on materials modelling, using discrete and continuum models.
- New exploitation channels for European academics and research organisations, in particular marketplace-based ones.
- Extension and upscaling of commercial software into modelling platforms well-suited to industrial application.



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### Current status:

We have identified a prototype to be demonstrated in one of the industrial partners.

### To be done:

Integration of further codes, implementing EMMC-supported interoperability standards.

### Partners:

#### *Identified:*

3 academics, 2 SMEs (software, manufacturing), 2 RTOs, 2 industrial corporations

#### *Missing:*

All welcome, *manufacturing companies in particular*