

EMMC Task Group proposal

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Focus Area: *Model Development (also Software)*

Linking and Coupling Computational Chemistry to Electromagnetics

Task Group

Motivation: EMMC assembles groups active in the developments of different material model types and even more such models are available on the European research area. Typically, each model comes with its own user interface, and in many cases the model cannot be practically used by anyone except its authors. This hinders and often prohibits:

- exploitation of many outstanding research results,
- reliable comparisons of results from different models and / or solvers for a pre-defined benchmark,
- linking and coupling of models of different categories.

The goal of the *Models Linking and Coupling* Task Group is to address the above problems and **improve the interoperability** within different material modelling levels, which will allow for **increasing industrial impact** of the actions undertaken by EMMC ASBL.

The proposed methodology is to develop and share a common, interoperable graphical user interface (GUI), allowing for launching dedicated, advanced modelling tools. Such an approach will deliver a complete solution allowing for **multi-scale multi-physics material analysis** from the **electronic** level, through **atomistic** and **mesoscale** to **continuum** modelling (and possibly also **data-based modelling**), which eventually enables the **analysis of device performance**, being of high **interest of industry**.

Enhanced visibility to the material modelling activities in general, and specifically to hierarchical modelling, and models linking and coupling, will be achieved.

The planned result is a modelling platform with **common, interoperable GUI** and a **built-in library of User Cases**, corresponding models and solvers which will:

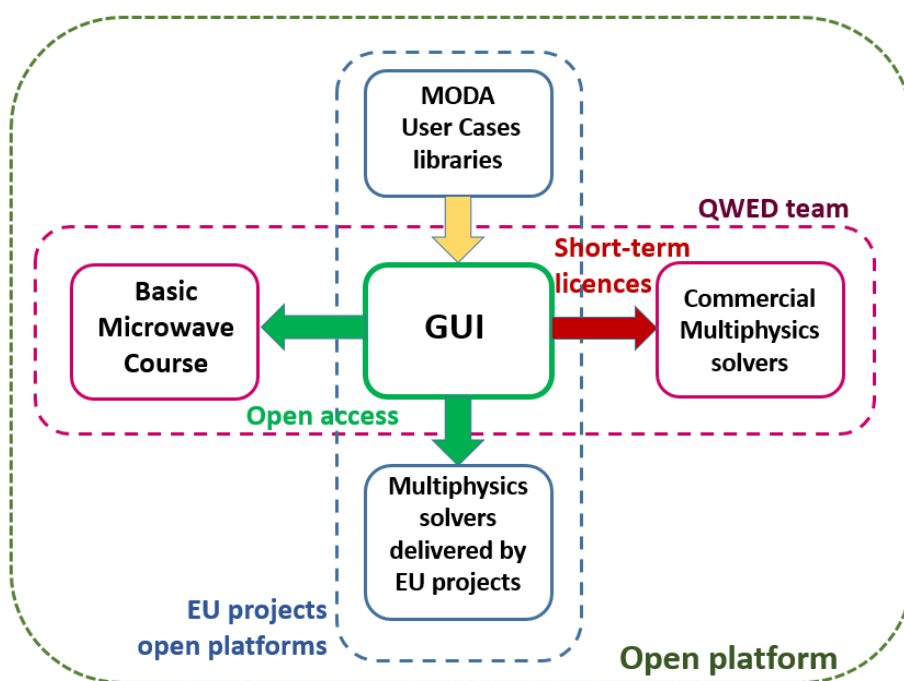
- eliminate the necessity of conducting expensive process of **learning different GUI tools**, typically accompanying solvers dedicated to different model categories,
- eliminate the necessity of an even more expensive process of **setting up a new GUI**, for a model that has been successfully used by its authors by brute-force (e.g. entering data into a source code),
- maintain a **common library of User Cases**, as recommended by *RoMM V*, for which models of different categories can be set up and **cross-verified**,
- facilitate easy **choice of the most adequate model** category for each User Case,
- facilitate **switching** from the fastest to solve **continuum models**, all the way down to the most accurate **electronic models**, when appropriate computer resources become available,

- facilitate **defining linked and coupled modelling workflows**, comprising the models and solvers available on the modelling platform,
- make the **User Cases** and their models **FAIR** (findable, accessible, interoperable, reusable).

The proposed **Access Rights** to the platform will be as follows:

- the **GUI** will be **licence-free**, available to anyone worldwide on Controlled Licence Terms,
- the core library of **User Cases** will be **free** but **expandable** with both free and licensed examples,
- a **set of open** (but not necessarily open source) **models** and **solvers** will be provided,
- **interfaces to selected commercial software** will be provided.

A schematic access rights diagram, with exemplary commercial contribution of QWED, is presented by the below picture.



The **industrial impact** of materials modelling will be enhanced, delivering an **access point** for commercial modelling and translation services.

The **Models Linking and Coupling Task Group** will merge interests of Focus Areas of EMMC:

- **Interoperability**
- **Model development**
- Software deployment
- Industrial impact

Starting point and actions

Note: implementing a new GUI from scratch is an effort estimated in man-years of work, even when some well-known graphical libraries are used. It is therefore beyond the scope of this Task Group. Our proposal therefore is to start from an existing GUI, which itself is a workbench for FreeCAD libraries, and to focus on adding functionalities needed for the models and solvers of the Platform.

To get started, open GUI (licence free), being under development (by QWED) within H2020 MMAMA project (and currently under further development and enhancement towards battery modelling in H2020 NanoBat project), can be considered. As a deliverable of the MMAMA project, the GUI will enable launching free FDTD and FEM electromagnetic solvers and coupled electromagnetic-semiconductor solver resulting from MMAMA, as well as commercial multiphysics solvers of QuickWave family.

The *Models Linking and Coupling* Task Group will **take actions and deliver recommendations** for:

- **adapting the GUI** of physical continuum models to those of different categories (**electronic, atomistic, mesoscopic**) and also to data-based models,
- **promote** the idea of building/creating the interfaces between commercial and academic modelling software and the open GUI to **enhance the software deployment and interoperability**.