D3.3 TWO OPEN PLATFORM TOOLS (STANDALONE TOOL AND GUI) AND ONE EXAMPLE FOR TIP-SAMPLE INTERACTION IN EMPRO

Contractual delivery date:	M34
Actual delivery date:	M34

DOCUMENT INFORMATION

Version	VF	**Dissemination level**	PUB
Editor	Arif GUNGOR - ETHZ		
Other authors	Malgorzata CELUCH and Janusz Rudnicki - QWED Jasmin SMAJIC – ETHZ Ferry KIENBERGER - KEYSIGHT		

PROJECT INFORMATION

Grant Agreement n°	761036
Dates	1st November 2017 – 31 October 2020

DOCUMENT APPROVAL

Name	Position in project	Organisation	Date	Visa
K. Haddadi	Coordinator	IEMN		

DOCUMENT HISTORY

Version	Date	Modifications	Authors
V1	26/08/20	Deliverable writing	M. Celuch
VF	31/08/20	Update of the document	A. Gungor, F. Kienberger

TABLE OF CONTENTS

1 EXECUTIVE SUMMARY

1.1 Description of the deliverable content and purpose

The main objective of MMAMA WP3 [1] is to bridge the gap between the capabilities of the currently available simulation technologies and the specific requirements of SMM, as well as those of other material measurement techniques considered in the project. The aforementioned "gap" is considered from two perspectives:
- the basic "technology gap", concerned with the availability of modelling tools and their validation in the subject area,
- accessibility of existing tools, not only in terms of their costs, but also awareness of their functionalities and competencies of use.

To locate MMAMA's modelling work in the context of EMMC activities [2] and MODA terminology of the EC *Review of Materials Modelling* [3], the following aspects must be highlighted:
- MMAMA WP3 is concerned with **physics-based models** (Fig. 1). This means that physics equations (PE) are combined with material relations (MR) into a system solved simultaneously and emulating real-life processes. This is opposed to data-based models, where the material or process behaviour would be deduced from earlier measured or simulated data sets, by interpolation, extrapolation or more complex artificial intelligence systems.
- Our models are **continuum**. This means that the model entity essentially is the continuum (as opposed to individual particles like atoms or electrons in discrete models). Nevertheless, in order to be solved on a computer, the model equations are discretised, i.e., written up for finite volumes (called elements or cells) over which the considered fields and material parameters are averaged. This leads us to finite element (FE) and finite-difference (FD) schemes.
- More specifically, our main models are electromagnetic (EM), governed by Maxwell equations, mostly in GHz frequency range. Coupled EM-semiconductor models are also considered. More details of our PE and MRs are given in the MODAs for the User Cases (UCs), see Section 2.6.
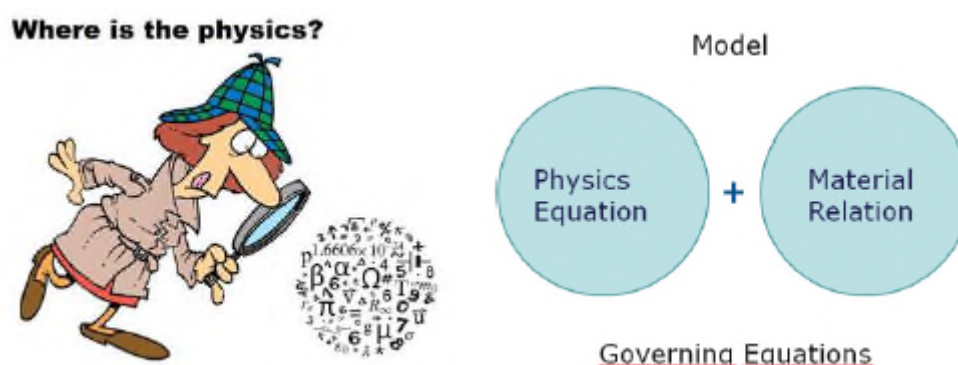

Fig.1: Concept and components of a physics-based material model after [3].

Throughout the project, physics-based models were being developed and validated for User Cases representative of SMM, dielectric resonator, and coaxial probe measurements of microwave material characteristics. The models were simulated with three groups of solvers, taking advantage of pre-existing knowledge of the partners embodied in:

- **ETHZ** in-house FEM solvers [4],
- **QWED** FDTD solvers of QuickWave family [5],
- **KEYSIGHT** FEM solvers in EMPro [6].

Moreover, ETHZ FEM tools and QWED FDTD tools were being extended with new models and procedures, for enhanced accuracy and computational efficiency in the considered applications. Modelling results of ETHZ, QWED, and KEYSIGHT are published in open access, see specifically [7]-[11]; also [1] and [12] for further references.

While MMAMA modelling validation and development works were performed to narrow the "technology gap", **Task 3.4 reported herein addresses the other identified gap, namely, that of models' accessibility. It delivers Open Platform tools and examples, serving two main purposes:**
- **dissemination of the project results,** demonstrating the relevance of GHz modelling to materials research and characterisation in industry,
- **education in the use of materials modelling**, facilitating acquisition of modelling and simulation skills by students and engineers.

According to MMAMA, the Open Platform was planned to include:
   a) a workbench based on the FreeCAD library for setting up CAD models of tip-sample interactions (by QWED),
   b) a standalone application which enables simulation of tip-semiconductors in a parameterised way (by ETHZ),
   c) a tip-sample example in EMPro for solar cells (by KEYSIGHT).

The above goals have been reached, and further functionalities have been added:

   a) A workbench based on the FreeCad library for setting up CAD models of tip-sample interactions has been developed by QWED and provided open-access under the name MMAMA-Modeller [12]. Its installation includes QWED FDTD solvers, which are licence-free versions of QuickWave solvers, including the new features developed within MMAMA. Also an added functionality is, that MMAMA-Modeller allows automatically launching ETHZ FEM solvers and visualising FEM results, in a manner compatible with FDTD visualisation. MMAMA-Modeller is described in Section 2.1.
   b) A standalone application which enables simulation of tip-semiconductors in a parameterised way has been developed by ETHZ. Time- and frequency-domain solvers (TD-FEM and FD-FEM) are adapted to the Open Platform. An added functionality is, that the FDTD mesh generated by MMAMA-Modeller is imported and converted into FEM mesh, whereupon FEM simulations run automatically, and the results can be displayed in the common GUI, as described in Section 2.2.
   c) A tip-sample example in EMPro for solar cells has been programmed by KEYSIGHT. It is described in Section 2.3.

Section 2.4 presents FDTD and FEM simulations of an SMM tip interacting with a sample example, defined in MMAMA-Modeller. Sections 2.5 and 2.6 summarise the current contents of the Open Platform and its extensions scheduled within MMAMA. Conclusions refer to the Open Platform use and developments beyond the project lifetime.

4

1.2   Brief description of the state of the art and the innovation breakthroughs

Electromagnetic modelling long ago gained large popularity with the microwave community. Its use for practical design of microwave components was pioneered in 1980s, and full systems can be analysed with fully-fledged EM software. There is a proliferation of in-house customised tools (of which the on-going research of the ETHZ team members and the original research of QWED founders are representative) as well as a number of general-purpose well-validated commercial EM packages (of which EMPro and QuickWave are good examples). Although it may sound cliché, we wish to note that the two approaches (in-house and commercial) **have their own advantages:**

- The **commercial tools** are equipped with user-friendly interfaces, providing flexibility of defining a broad range of structures, convenient displays of results, and typically also parameterisation functionalities.
- The **in-house tools** allow their authors to internally adjust simulation parameters (e.g. meshing) for best accuracy in a particular simulation. They are also relatively easily adapted to specific requirements of a new scenario.

The first innovative aspect of this Deliverable consists in combining the advantages of in-house and commercial modelling tools:

- On the one hand, the developed MMAMA-Modeller allows easy definition of model geometries and parameters, in a manner compliant with popular 3D CAD approaches. The models can be parameterised and easily re-run by FEM and FDTD. A convenient graphical user interface (GUI) is also provided for displaying simulation results. These developments within the project were made possible by QWED earlier experience with its commercial QuickWave software.
- On the other hand, MMAMA-Modeller, FEM, and FDTD solvers are maintained as separate applications, communicating through text-files. This allows model modifications and manual tuning by software authors or advanced users.

In essence, all EM modelling tools solve the Maxwell equations subject to particular boundary conditions (BCs) and excitation. Maxwell equations are 4D equations (differential or integral), in 3D space and time. By virtue of the Fourier transform, the time variable can be converted into frequency. This gives the basis for the **frequency domain (FD) methods**, where the 3D problem in space is solved for a particular value of frequency. In the alternative **time domain (TD) approach**, the time variable is discretised, and the numerical solution is marching-in-time. Both FD and TD have their advantages and disadvantages; for example, TD provides a wide frequency band response after a single simulation, but suffers from long convergence when applied to high-Q problems. The opposite is true for the FD approach.

The second innovative aspect of this Deliverable is, that both TD and FD tools are provided and previously benchmarked against each other, in the cases where both approaches are applicable [8][11][15].

It can be argued that there exist commercial software packages, where both TD and FD solvers are included (see Section 2.3). However, capabilities of different solvers may be difficult to compare in a fair and exhaustive manner, as their functionalities do not need to be the full functionalities of the corresponding modelling method, but rather, arbitrary choices of the vendor's implementation. Moreover, interfaces within commercial packages are typically

5

confidential, and their providers have no interest in facilitating direct comparisons to other forthcoming tools.

The main therefore innovative aspect of this Deliverable is, that it is open to the research community and collaborations are encouraged:

- The formats of files (exported by MMAMA-Modeller and input files of the solvers) are open, so that other models and solvers can be connected to the platform, and also mutually benchmarked.
- Last but not least, the Platform is free to use, which is expected to generate more feedback and stimulate its future extensions.
- The MMAMA Open Platform has already been subject of presentations and papers in the relevant communities [13][14][15] and further dissemination is scheduled, e.g., Short Course at MIKON-2020 Conference and session at EMMC International Workshop 2021. This aspect is addressed in Section 2.6.

1.3   Corrective action (if relevant)

N.A.

1.4   IPR issues (if relevant)

Relation to Background:
The original modelling methods and solvers constitute the Background Knowledge of ETHZ, QWED, and KEYSIGHT. In accordance with the H2020 rules and the Consortium Agreement, nothing in the project changes those IPR ownerships.

Generated Foreground:
The modelling results of this Deliverable remain the property of the partner who has generated them. Representative results have been published and are available as open access [7]-[15].

Besides the simulation results, the generated Foreground includes new software items:
- **new EM models** (e.g. ETHZ coupled Maxwell-semiconductor model, for the modelling of drift-diffusion influence of SMM measurements),
- **new EM modules** (e.g. QWED double-precision implementation of QW-Simulator, for higher-accuracy de-embedding the influence of SUT on capacitance seen by the tip).
The models and modules implemented by the partners, beyond the published information, remain in the partners' repositories for future commercialisation.

2   PURPOSE

2.1   MMAMA-Modeller developed by QWED with built-in FDTD solvers

MMAMA-Modeller is a licence-free CAD modeller developed within the MMAMA project designated for analysis of axisymmetrical Bodies of Revolution (BOR) structures.

QW-Modeller permits CAD definition of 3D structures, mesh generation, and specification of simulation parameters via a convenient system of dialogue boxes.

QW-Modeller for QuickWave is a plug-in (workbench) for the open source *FreeCAD* (http://www.freecadweb.org), general purpose feature-based parametric 3D CAD modeller with a modular software architecture, which makes it easy to provide additional functionalities without modifying the core system. The CAD capabilities of *FreeCAD* are based on the OpenCasCade® kernel, a professional-level CAD kernel, featuring advanced 3D geometry manipulation and objects.

MMAMA-Modeller is free and can be used without any restrictions for creating geometry, assigning the materials, adding ports, boundary conditions, setting mesh, excitation parameters, postprocessing etc.

MMAMA-Modeller automatically generates conformal FDTD mesh. The user is equipped with many means of controlling the meshing process, including the enforcement of global and local maximum cell size, mesh snapping planes, mesh refinement in regions of expected rapid field variation and *AMIGO* (Automatic Meshing Intelligent Generation Option). The following aspects of the mesh generation are important for the general-purpose use of MMAMA-Modeller by different FDTD and FEM solvers:

·   the primary generated mesh is conformal FDTD mesh proprietary of QuickWave software by QWED,

·   the mesh is exported in text files of an easy *sh3 format, allowing its conversion to other spatial meshes, e.g., classical stair-case by eliminating non-standard cells,

·   an example of mesh transformation is ETHZ software, included on the Platform, which detects FDTD mesh vertices and edges and trangularises into the desired FEM mesh.

MMAMA-Modeller allows preparing a complete project for electromagnetic simulation with:
· user-friendly CAD environment for complex geometry definition,
· easy-to-learn set of tools,
· complete electromagnetic simulation definition,
· EM sources, field monitors, boundary conditions,
· postprocessing tasks: S-parameters, antenna pattern, power available etc.,
· Automatic Mesh Intelligent Generation Option (AMIGO), with mesh controlling tools,
· material parameters,
· parameterised geometry.

More detailed information about *MMAMA-Modeller* is given in the *MMAMA-Modeller* help available by pressing *F1* key or by choosing *Help ® MMAMA-Modeller Help* from the main menu. In view of MMAMA-Modeller direct applicability to QWED FDTD tools, its help files are identical to QW-Modeller files).

More detailed information about *FreeCAD* is available on the *FreeCAD* website (http://www.freecadweb.org) or in the *FreeCAD* help through *Help ® FreeCAD Help* from the main menu.

Note that due to FreeCAD use, most dialogues and command names appears in the language of the user's operating system (Polish in the example dialogue of Fig. 2).
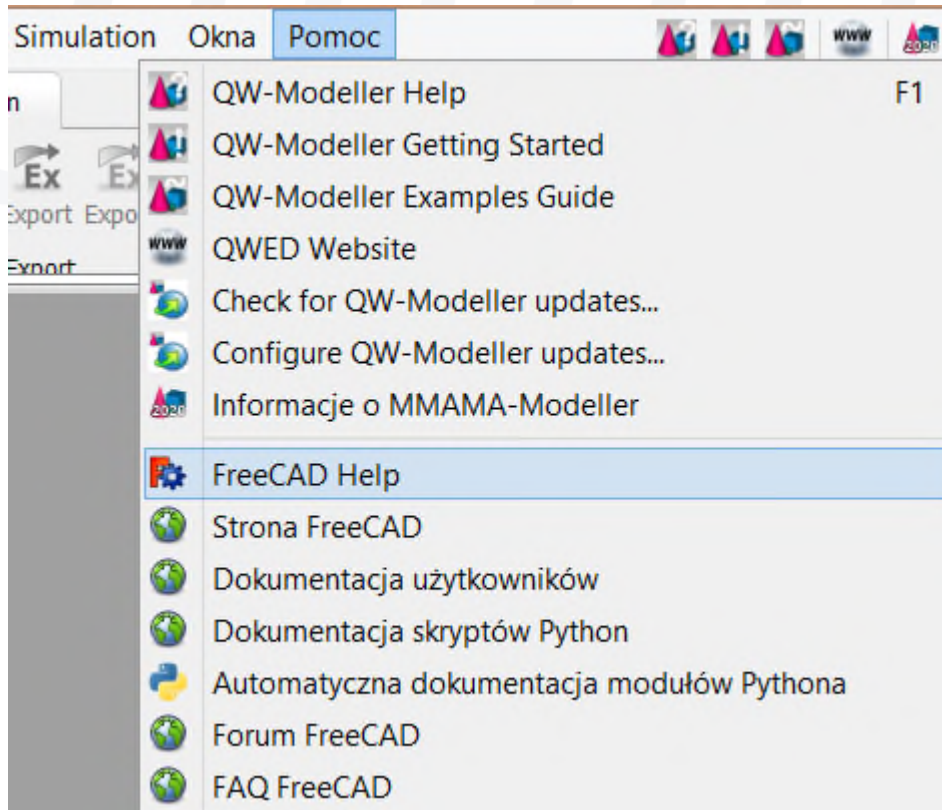

Fig.2: "Help" dialogue of MMAMA-Modeller as it appears on a PC with the Polish version of the operating system.

Parametrisation in MMAMA-Modeller

Parametric modelling can be used in MMAMA-Modeller for designing parametrised models by using user defined variables.
The *Model* tab in the ribbon contains *Parameters* section with *Parameters* button for opening/closing of QW-Parameters dock window that allows defining user variables.

All user variables will appear in the Tree View under User Parameters group.

8
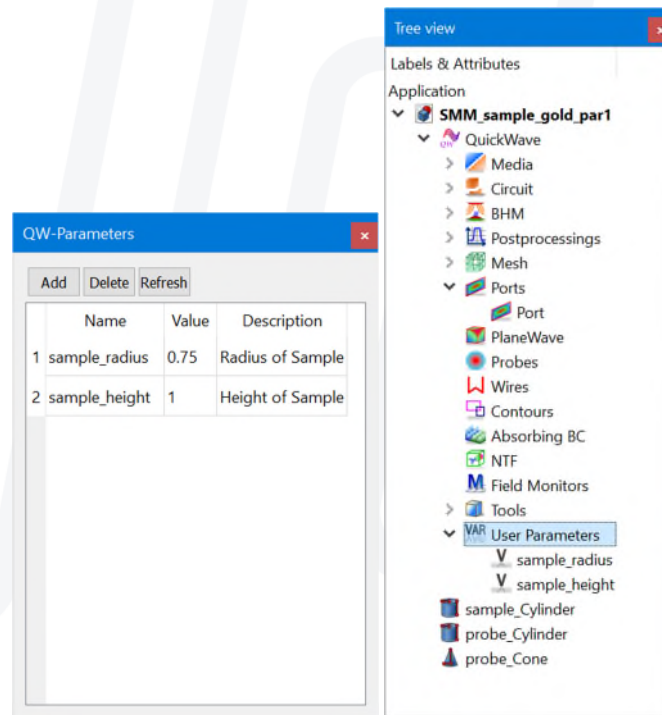
Fig. 3: Parameterisation dialogues of tip-sample example in MMAMA-Modeller.

User variables can be used for geometrical objects (i.e. 'sample_radius' variable is used for radius of sample's cylinder).
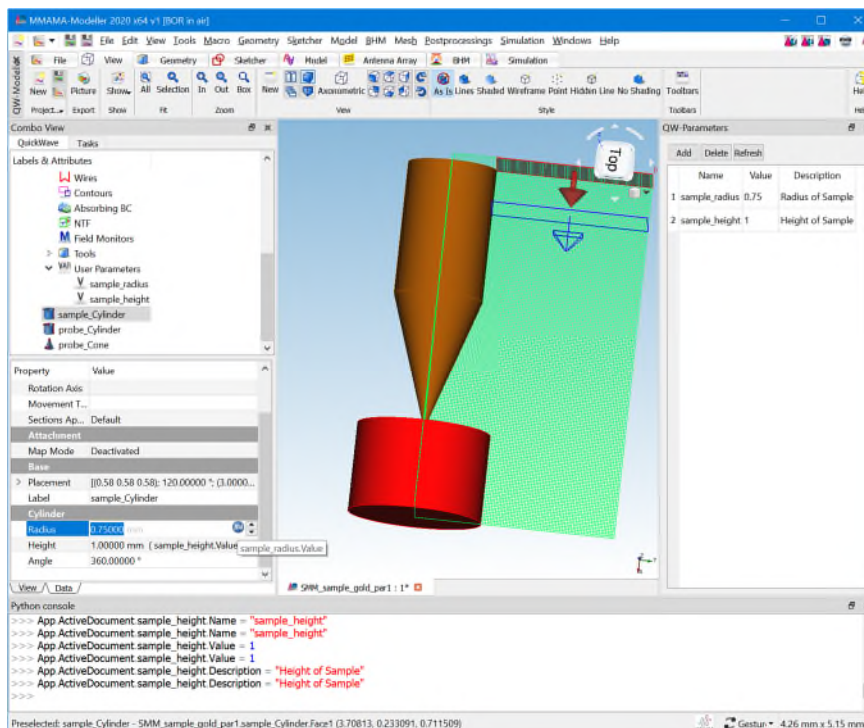
Fig. 4: A parameterised tip-sample example in MMAMA-Modeller: before tip radius change.

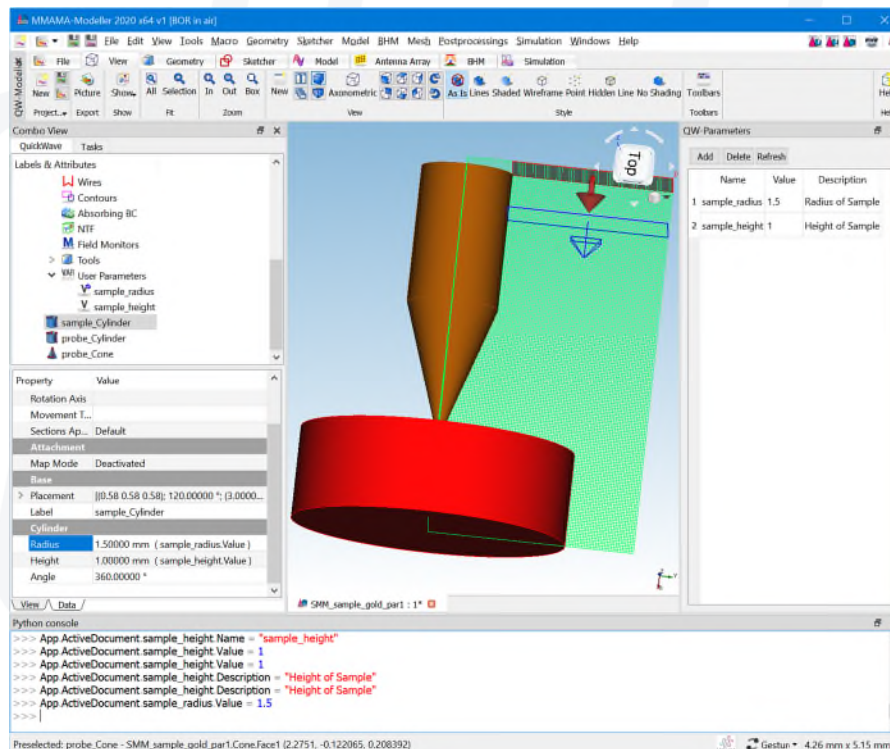The change of value of 'sample_radius' variable causes the change of the radius of the sample's cylinder.

Fig. 4: A parameterised tip-sample example in MMAMA-Modeller: after tip radius change.

2.2 FEM solvers developed by ETHZ and integrated within MMAMA-Modeller

Finite Elements Method (FEM) is a numerical method to obtain approximate solutions to boundary value problems of engineering and mathematical physics. Three types of FEM solvers have been developed in MMAMA:

A. EM BOR FEM solvers in Time Domain [8]
B. EM BOR FEM solvers in Frequency Domain [8][11]
C. Coupled Maxwell-semiconductor BOR FEM solvers in Time Domain [10].

In Task 3.4, it has been decided that EM BOR FEM solvers in time- and frequency-domain will be provided on the Open Platform, for the purposes and dissemination and teaching. The coupled Maxwell-semiconductor solver has a highly competitive potential and as such, will be restricted to further competitive use by ETHZ.

MMAMA-Modeller is integrated with FEM solver developed by ETH Zurich and allows FEM simulations directly from *MMAMA-Modeller* GUI.

The *Simulation* tab in the ribbon contains *FEM Simulations* section with commands for preparing, launching and viewing FEM simulation results:

Ex FEM Export - opens *FEM Simulation* dialogue and starts FEM export with the FDTD-FEM mesh converter
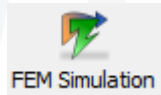
FEM Simulation - opens *FEM Simulation* dialogue and the Time Domain Maxwell solver based on Finite Element Method

FEM View - opens for visualization (in QuickWave Simulator) CSV files with EM fields from the FEM simulation
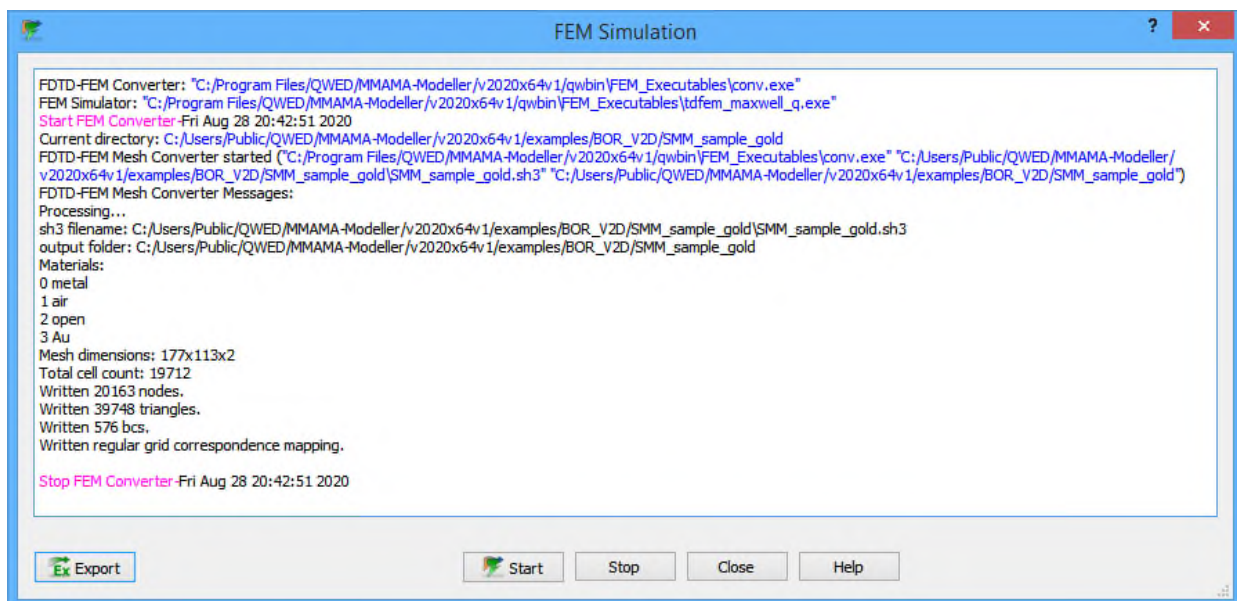
FEM Help - opens help for FEM simulations

Fig. 6: *FEM Simulation*, as displayed within the MMAMA-Modeller main window.

FEM simulations workflow:

1. Export FDTD mesh

2. Start the FDTD-FEM mesh converter:

- reads in rectangular FDTD mesh and converts it to triangular FEM mesh

3. Start the Time Domain Maxwell solver based on Finite Element Method:

- reads the triangular mesh that is based on the outputs of the FDTD-FEM mesh converter

the distribution for r component of the E- field saved to CSV file at every 10 time steps

the distribution for z component of the E- field saved to CSV file at every 10 time steps

produce other output files (transient port voltage V(t), transient excitation voltage, dft of the port voltage, real and imaginary part V(w)…etc.)

4. E- field saved to CSV file can be visualised in the QuickWave Simulator.

2.3 Tip-sample example in EMPro programmed by KEYSIGHT

KEYSIGHT approach to the tip-sample example has originated from its actual experience of the measurements of the same, with Keysight NAs and SMM probes. In SMM reflection mode, the VNA sends an incident microwave signal through a conductive cantilever tip. The AFM cantilever is used to probe the local signal reflected by the sample while the VNA measures the scattering parameter S11 for standard reflection mode imaging. The reflection signal is based on the impedance variations caused by the electrical properties of the sample, S11=((ZL-Z0))/((ZL+Z0)), with ZL being the load impedance and Z0 the characteristic impedance of the line. An important step for quantitative SMM imaging is the calibration of the S-parameters to get the sample impedance Z. To better understand the measurement principles and the calibration procedure the local nanoscale tip-sample interaction needs to be modelled. For this reason, the use of FEM within EMPro as a tool to investigate and understand nanoscale phenomena.

A 3D example representative of an SMM tip is a contact with a sample; it has been programmed by KEYSIGHT in EMPro software and studied in the project. For the modelling, a 3D-field solver (FEM) in EMPro was used to model S11. The micrometric parts of the probe-sample system were transferred in a CAD (computer aided design) design and modelled in 3D using the electromagnetic finite-element model and the corresponding FEM solver of EMPro. All EMPro simulations were carried out in full-wave EM simulations.
Actually, there are two simulation engines available in EMPro: FEM and Finite Difference Time Domain (FDTD). Here, we used FEM simulations because of the availability of waveguide ports in EMPro, which are useful for the examination of components with unknown wave propagation modes, and because of the flexible meshing algorithms of the FEM solution. The first step in setting up an EMPro model is to create the 3D geometry and define the materials and corresponding properties. The 3D model can be either created by using different low-level geometric forms (e.g. cylinders, cuboids, or frustums) or by importing a 3D CAD model (several file formats are accepted).

The considered CAD model of the probe-sample system is shown in Fig. 7 and consists mainly of the probe (defined as the AFM cantilever and the nanoscale tip) and a layered semiconductor sample with different silicon doped layers.

Advanced variants of the demo example and in-depth studies of tip-sample interactions have been performed in MMAMA project KEYSIGHT and will be included in the confidential deliverable D3.5. (NOTE TO FERRY, TASK 3.6 to be closed M36 with D3.5: - Build an EMPRO and ADS combined model for problems including semiconductors in reflection transmission and comparison to measurements M1-M36 (KEYSIGHT, 3 PM)
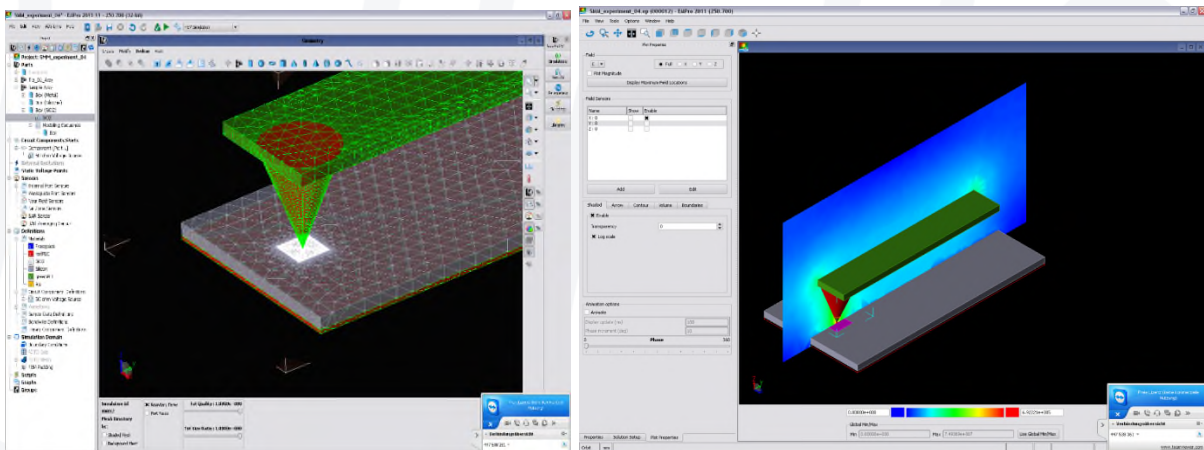
Fig. 7: The considered CAD model of the probe-sample system meshed in FEM (left) and the simulated E-field pattern (right).

More details on the setting up the SMM simulation in EMPro:
The tip-sample example, in its basic version, is included in the EMPro library of examples. As such, any EMPro user (including academic users of a short free trial license) can access the geometry file of the multi-layer sample. The below EMPro pictures with the tip on the multi-layer sample are taken directly from this demo-example. Modelling results relevant to the educational and dissemination purposes of this deliverable have been published in [10] and therefore, are already openly available.

The SMM demo project can be found in the Help/Examples menu. The examples are read-only files so it is useful to save a copy of the project for modifications. The parameter menu is selected with each parameter having its own short description. Parameters that are related to geometric objects are numbered from 1 upwards, while parameters intended for modifications are labeled by zero. Meshing of the tip-sample and numerical results, including complex impedance values. The simulations presented here are single-frequency simulations, but frequency sweeps are also possible. The second submenu provides several global parameters to control the meshing algorithm, while the third submenu allows selection of a direct or iterative solving strategy (here, iterative solving and quadratic base functions were used). Meshing can be controlled by individual mesh settings (which are independent for every part and include initial mesh size and meshing priority) and global mesh settings. Setting individual initial mesh sizes can help optimize the simulation time; different meshing priorities are useful to avoid meshing errors at overlapping areas (e.g., contact points). After setting the initial meshing, the refinement process starts. The mesh is iteratively refined and for every mesh a simulation result is calculated. The difference of the reflection coefficient of two consecutive simulations acts as the refinement exit criterion and a particular value can be preset. Regarding simulation time and memory, it took roughly 5 minutes on a standard desktop PC with a dual-core processor and 4GB RAM; the memory usage was roughly 2GB.

Figure 8 shows the nanoscopic tip-sample simulation of the cantilever and a three-layer stack sample, based on the EMPro SMM sample demo project. Geometric model of the cantilever, the probe tip, and the three-layer stack sample. The cantilever is 100 μm wide and 300μm long. The probe tip is modelled as frustum with an upper diameter of about 80 μm and a nanoscopic sphere as contact object at the bottom. The diameter of the very end of the probe tip is set to 20–100nm, which corresponds to a typical SMM tip diameter. Both the cantilever

13

and the tip are made of conductive platinum; therefore, they are modeled as perfect electrical conductors (PEC). The three-stack layer sample is composed of metal (red), doped silicon (10μm thick; dopant density 1017 atoms/cm3; conductivity 500S/m), and thin silicon oxide (50nm thick; relative permittivity 3.9). The bottom is a thin PEC layer representing the sample holder, which provides a return path for the RF current.
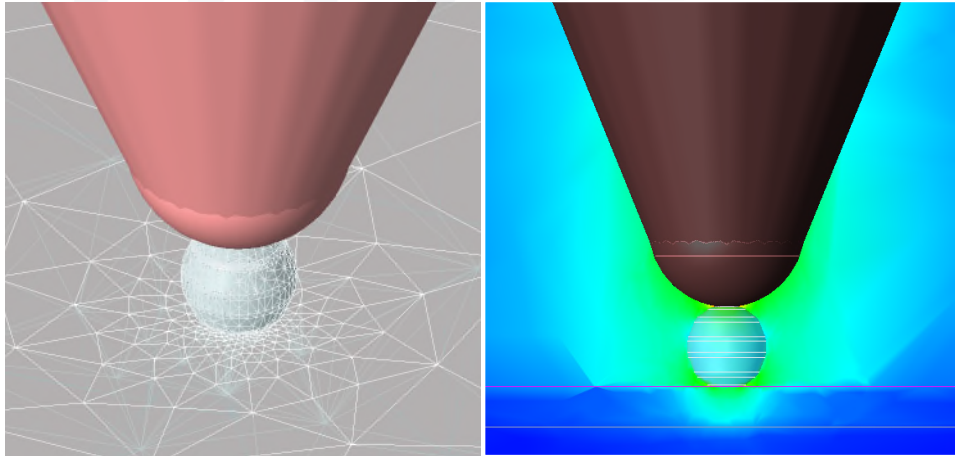

Fig. 8: Nanoscopic tip-sample simulation of the cantilever in EMPro.

2.4   Simulating a tip-to-sample example on the Open Platform

The *SMM_sample_gold.QWpro* model contains SMM probe modelling example prepared for FDTD as well as for FEM simulation.
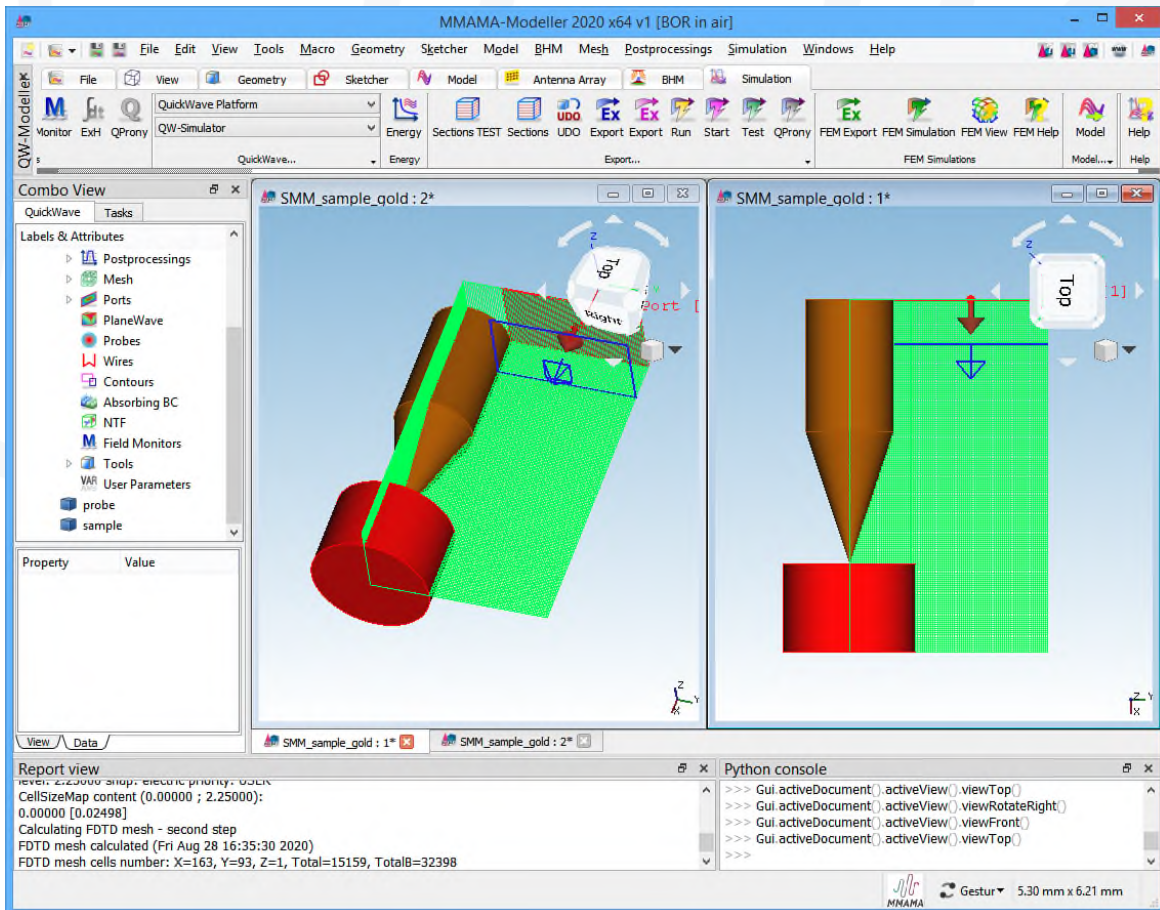
Fig. 9: SMM probe modelling example in MMAMA-Modeller.

The FDTD simulation in QuickWave can be started just by pressing Start button from *Simulation* tab. When performing the FDTD analysis in a wide frequency band, the S-

Parameters calculation results can be viewed by pressing Results button in QuickWave menu.
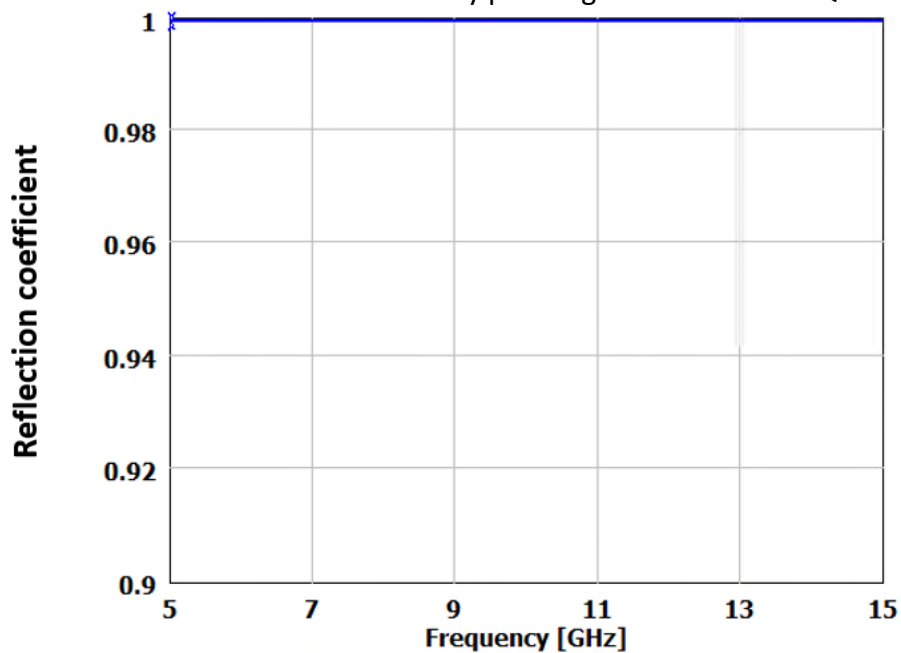
Fig. 10: S-Parameters from FDTD analysis for *SMM_sample_gold* example.

The distribution of the electric and magnetic field components can be investigated in real-time, while the simulation is running through **Fields** button or can be saved to file in CSV or GWYDDION formats.
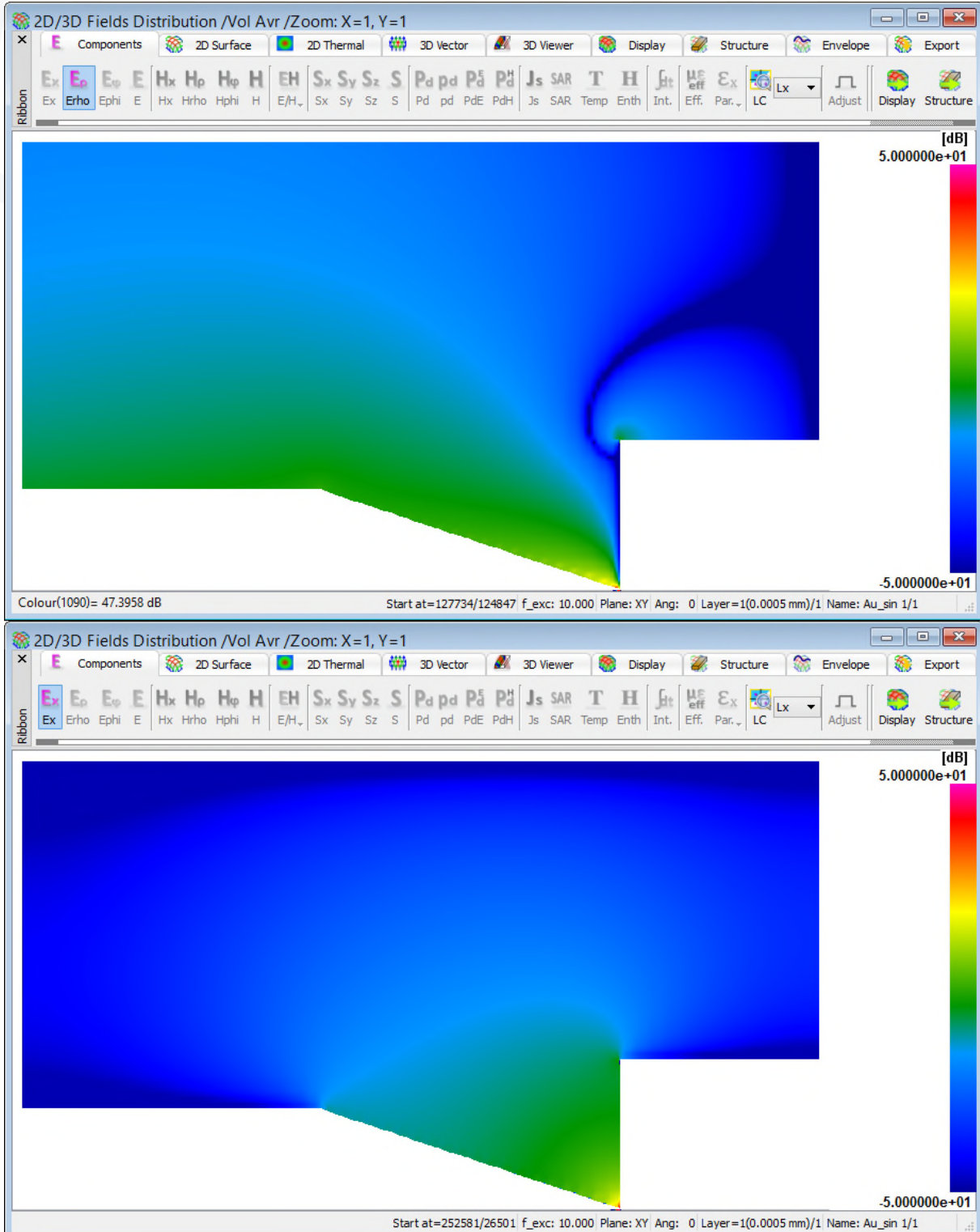
Fig. 11: Distribution of the electric field components (radial and longitudinal) in the *SMM_sample_gold* example obtained at 10 GHz from FDTD simulation.
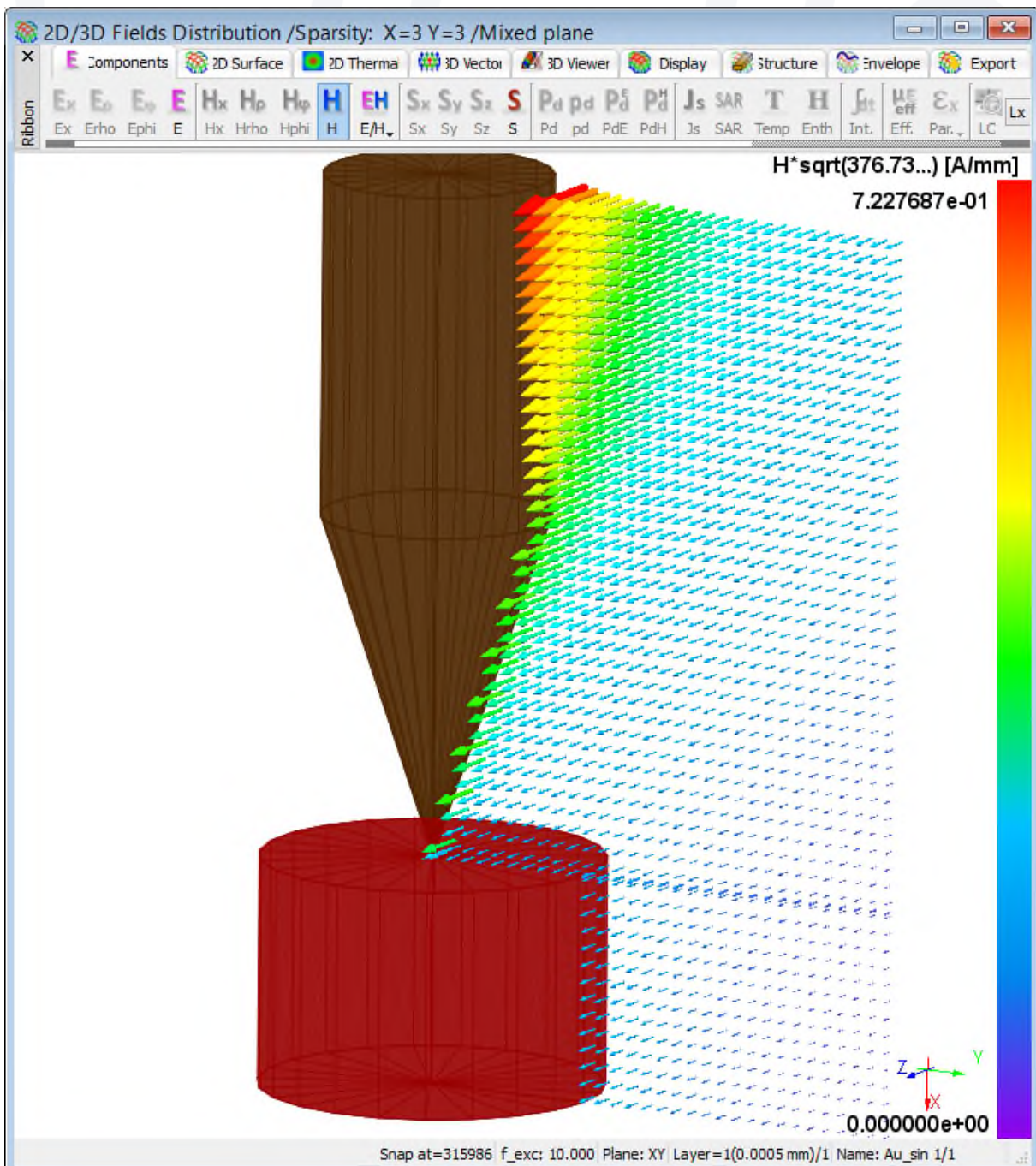
16

Fig. 12: Distribution of the magnetic field in the *SMM_sample_gold* example obtained at 10 GHz from FDTD simulatio.

The FEM simulation in Time Domain Maxwell solver based on Finite Element Method can be started according to FEM simulation workflow described above.

Start FEM export with the FDTD-FEM mesh converter by pressing in *Simulation* tab. FDTD-FEM mesh converter reads in rectangular FDTD mesh and converts it to triangular FEM mesh. The output information from FDTD-FEM mesh converter are displayed online in the *FEM Simulation* dialogue.
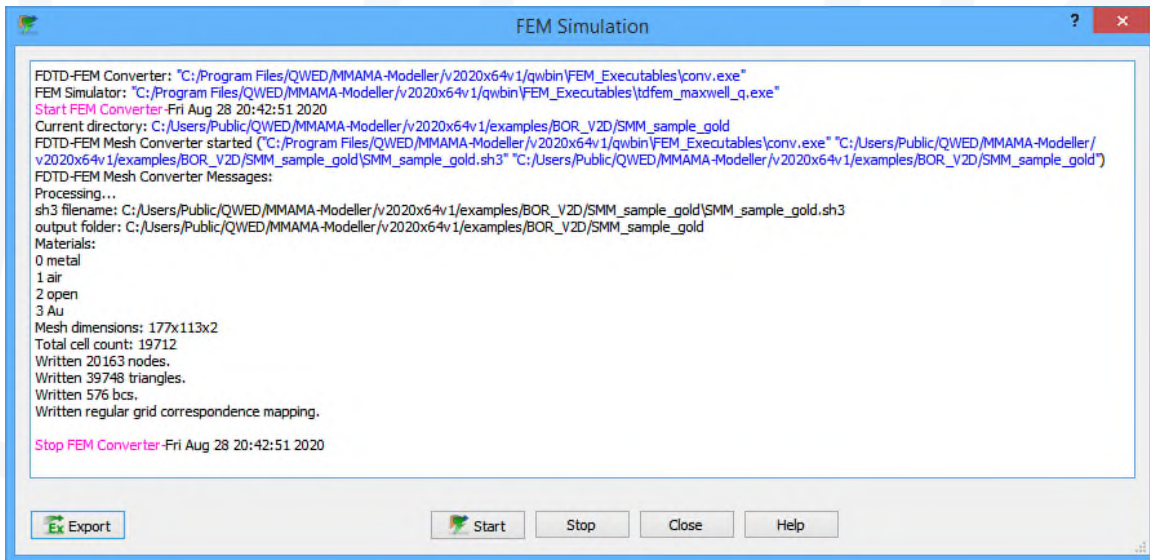
Fig. 13: Progress of mesh conversion from FDTD to FEM.

Start FEM simulation by pressing [Start] button in the *FEM Simulation*. It runs the Maxwell solver in the time domain and generates time-frequency domain signals and field profiles to be visualized at every 10 time steps. The output information from FEM simulation are displayed online in the *FEM Simulation* dialogue. The FEM simulation can be stopped by pressing [Stop] button in the *FEM Simulation* dialogue. In order to let the solver calculate complex S-parameters, one should let FEM simulation to finish itself.
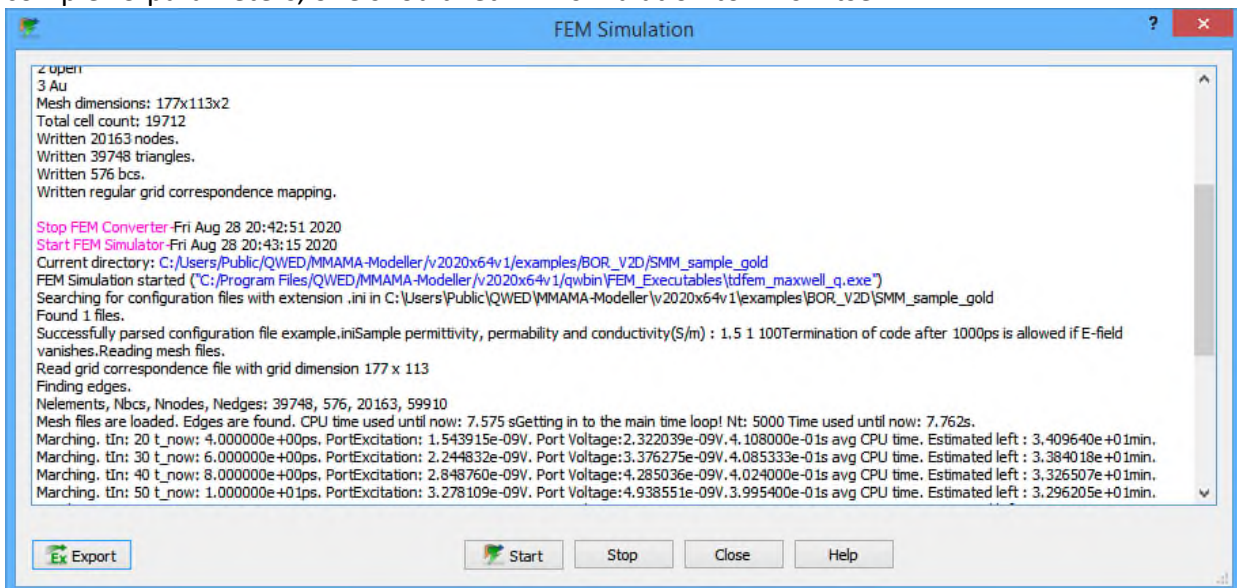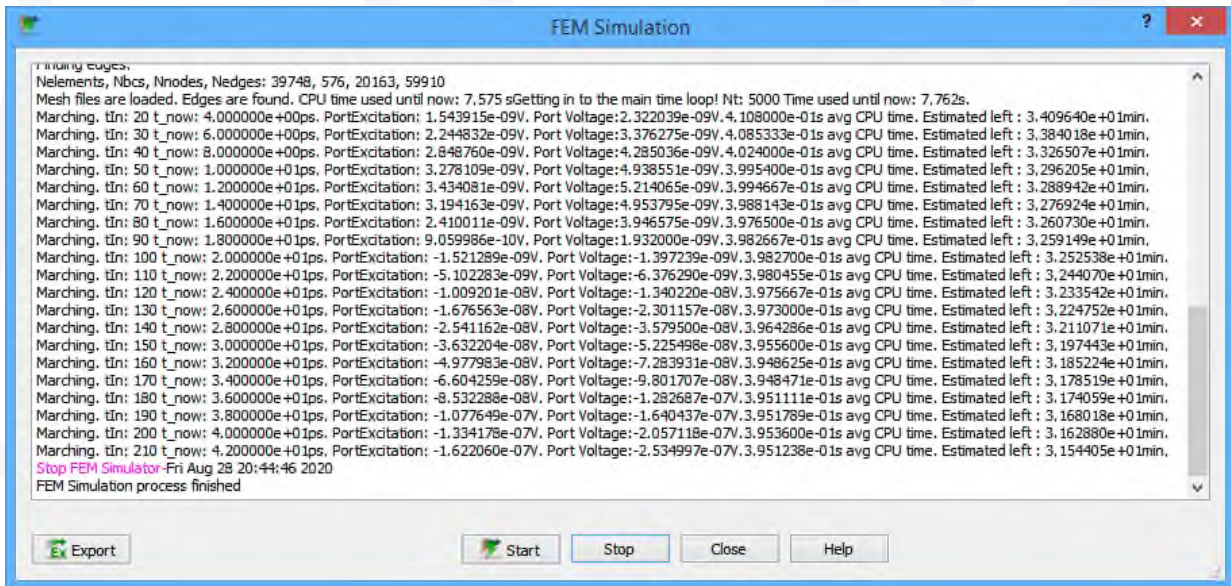
Fig. 14: Progress of FEM simulation.

The distribution for r and z components of the E- field were saved to CSV file at every 10 time step. CSV files with EM fields from the FEM simulation can be chosen and visualised in

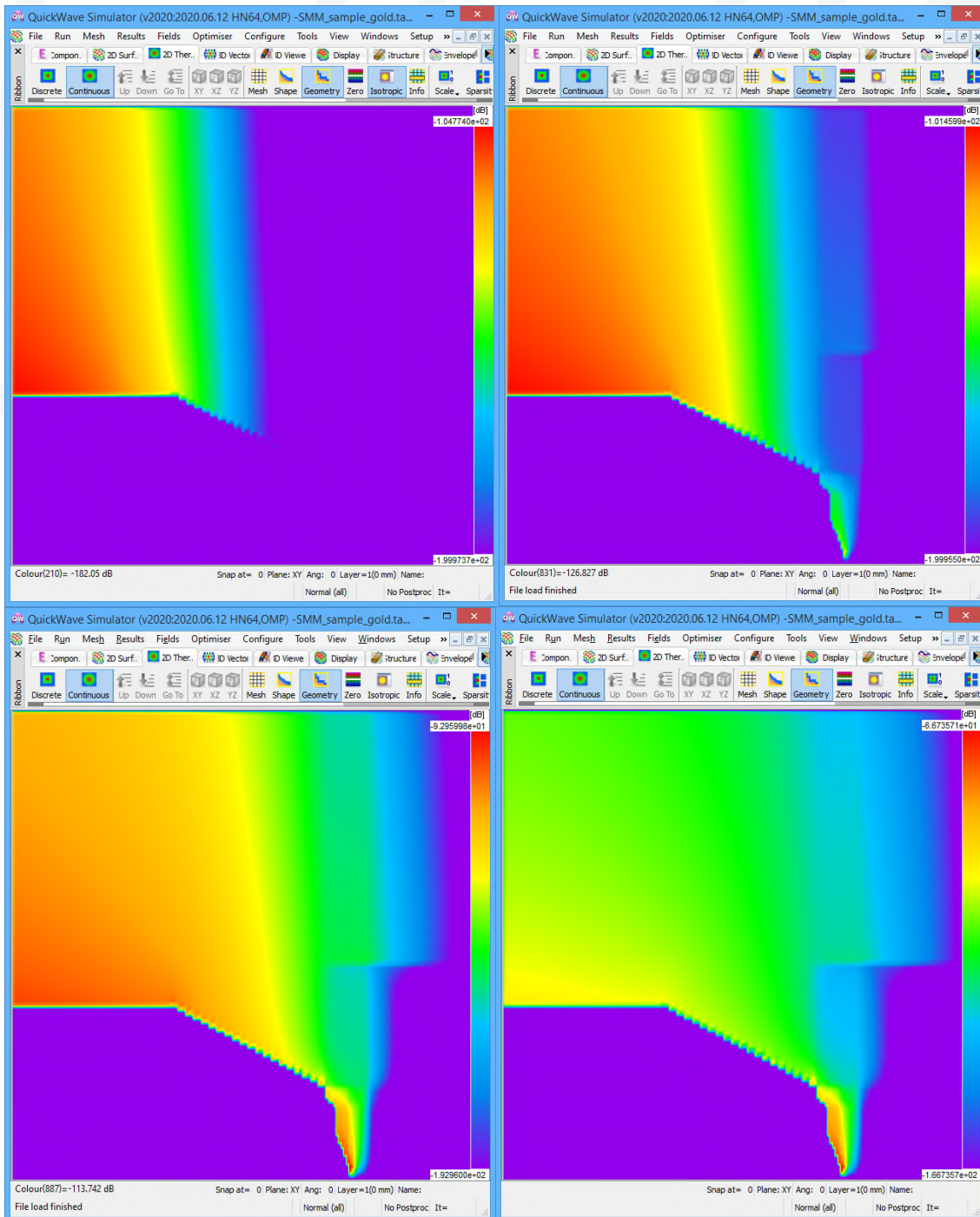MMAMA GUI by pressing button from *Simulation* tab.

Fig. 15: Distribution for radial component of the E- field at 20, 30, 40 and 50 time steps - visualisation in MMAMA GUI. (r- is vertical axis, z- is horizontal axis)
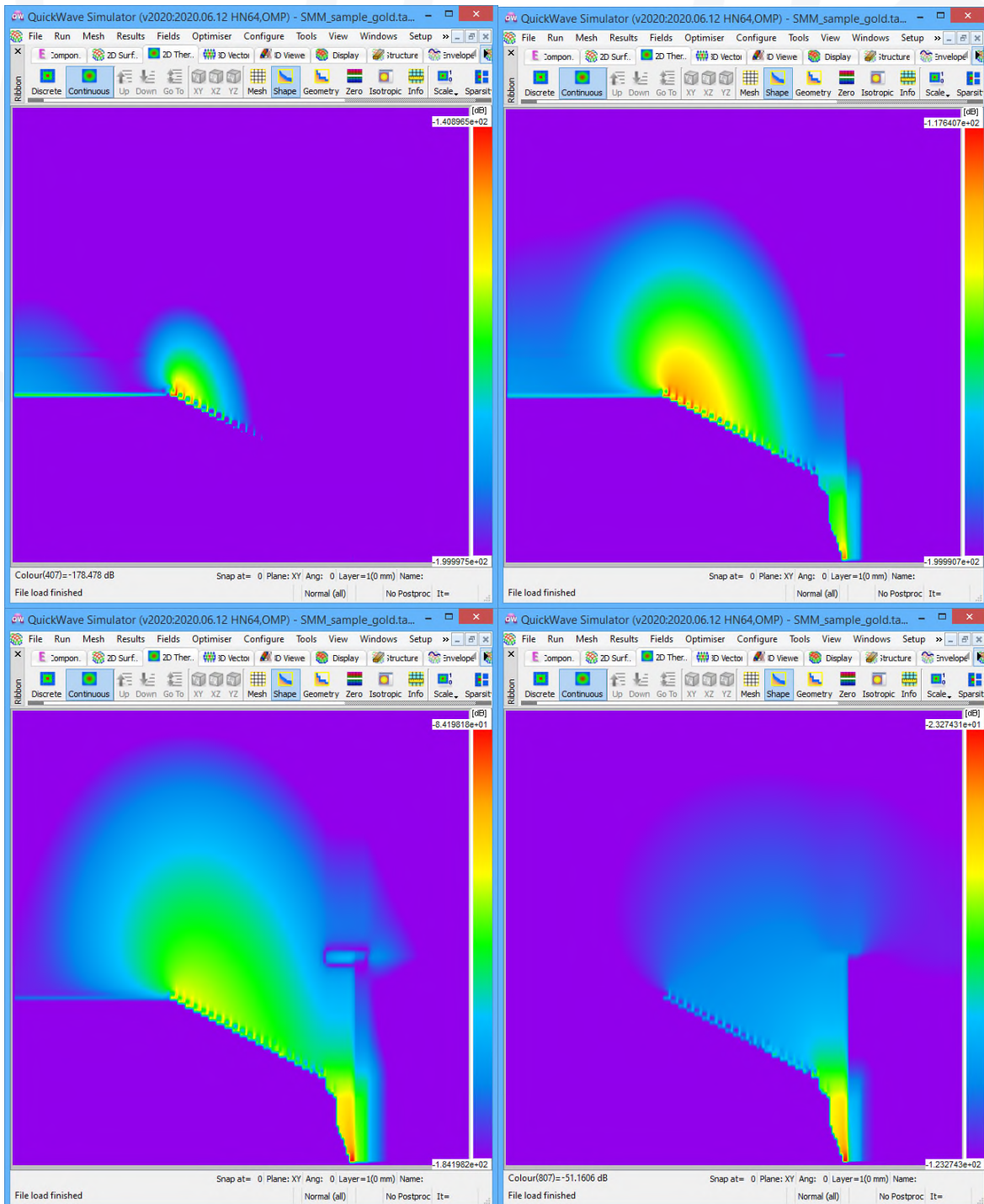
Fig. 16: Distribution for longitudinal component of the E- field at 20, 30, 40 and 50 time steps - visualisation in MMAMA GUI. (r- is vertical axis, z- is horizontal axis)

2.5   Open Platform: installation, content and hosting

The installation link for the MMAMA Open Platform tools and examples:
http://www.qwed.eu/QWUpdates/MMAMA_Modeller/v2020/MMAMAModeller2020x64.exe

The installation includes:
1.   MMAMA-Modeller

2. conformal BOR FDTD solvers
3. BOR FEM solvers - installed in directory qwbin/FEM_Executables
4. examples based on MODAs - in Version 1 of the Platform, there is one example (SMM_sample_gold: Permittivity and conductivity of the sample are parameterized and can be updated in the .ini file), additional examples coming in Version 2
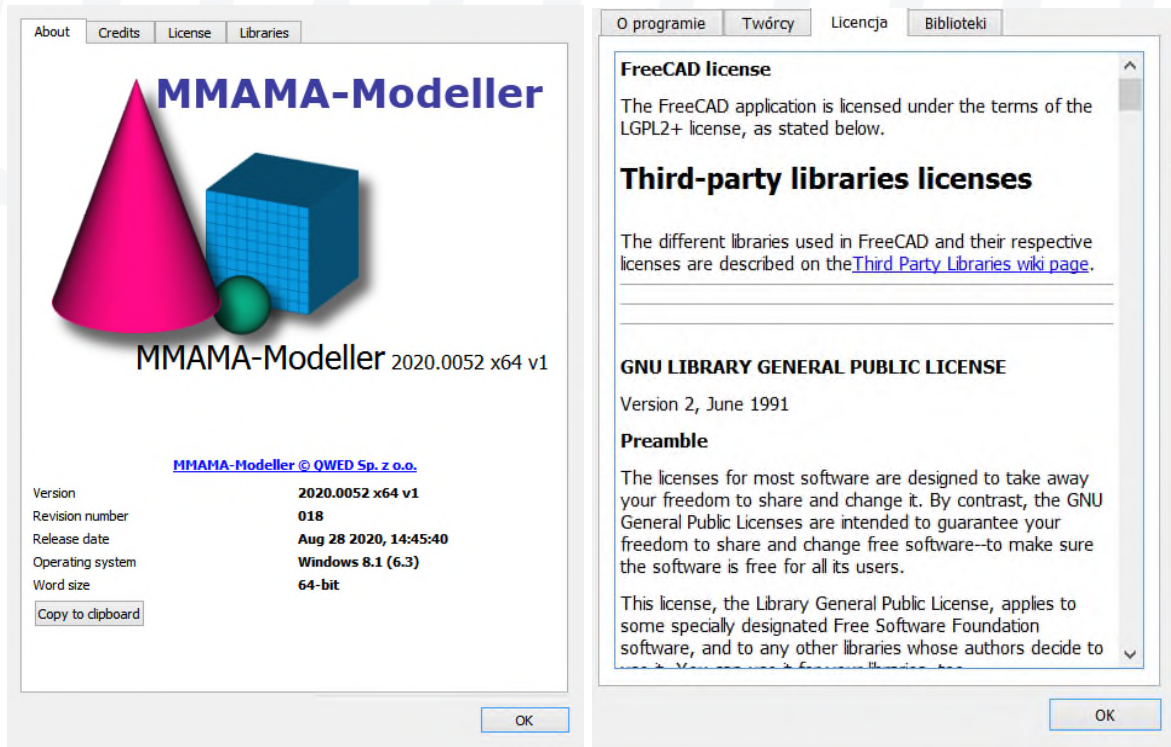

Fig. 17: "About" MMAMA-Modeller upon its installation.

As seen from the installation link, the Open Platform tools and examples are presently hosted on QWED website. Considering that the master module of the Platform, namely, MMAMA-Modeller, as well as the complete installation, have been developed by QWED, this arrangement allows QWED to dynamically react to any feedback from the MMAMA partners and to keep smoothly updating the contents until the end of the project.

Notwithstanidng the above decision, QWED is contractually bound to host the Open Platform tools and examples for at least 5 years after the project; taking into account the interest and collaborations initiated within the EMMC, QWED expects to host and maintain the Platform for much longer, including inputs from other projects and contributors.

While the Platform is visible to any visitor to QWED website, the installation link (with an explicit invitation to test and review the contents) has been sent to the projects partners. Invitations will be sent to sister projects (e.g. NanoBat) and EMMC members upon the release of this Delieverable.

2.6 Open Platform extensions planned during MMAMA and beyond

MMAMA Open Platform solvers are capable of simulating three User Cases, representative of the material measurement test-fixtures developed in the project, and described in the MODA format:
User Case 1: SMM tipe
User Case 2: Sapphire resonator supporting whispering gallery modes

User Case 2: Coaxial probe

User Case 1 is included in Version 1 of the Open Platform tools and examples; User Cases 2 and 3 will be uploaded before the end of the project.
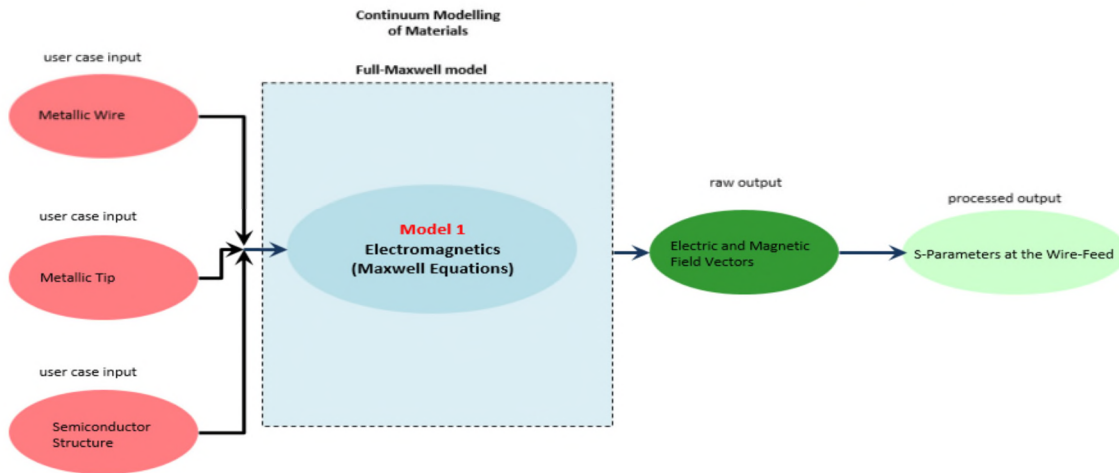
Fig.18: User Case 1: SMM tip (as discussed above; presented in [8][10]).
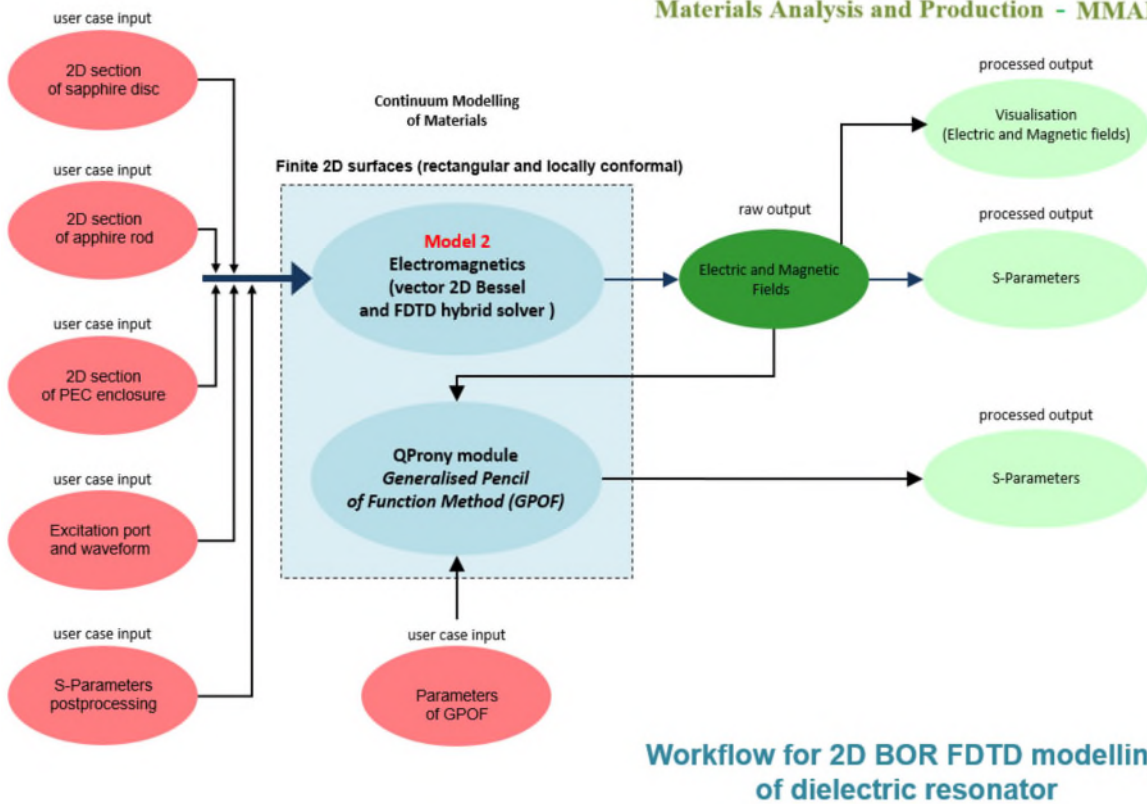
Fig. 19: User Case 2: Sapphire resonator (presented in [7][8]).

It is envisages that the MMAMA Open Platform becomes further extended with solvers and models, coming from the European projects and other contributions of the materials modelling community. The concept is presented in Fig. 20, where:

- *GUI* is the kernel of the Open Platform, assumed to be the current MMAMA-Modeller extended with features needed to activate additional models and solvers.
- *Physics-based solvers.* include the current MMAMA FDTD and FEM solvers, plus other solvers coming from EU projects or other initiatives, willing to provide their tools as open-access. Note that it is not necessary to provide open-source, as long as intermediate formats are preserved.
- *MODA* are User Cases libraries, documented in MODA formats.
- *Tutorials* are meant to help dissemination of the projects' results as well as teaching (such as QWED existing Microwave Course [5])
- Since GUI exports data in text files or easily documented formats, it will be possible for external **commercial solvers** to read and process the data. This creates a unique capability to run full-power simulations of examples created in the free-to-use GUI (note that commercial software typically does not allow running examples created in demo versions).
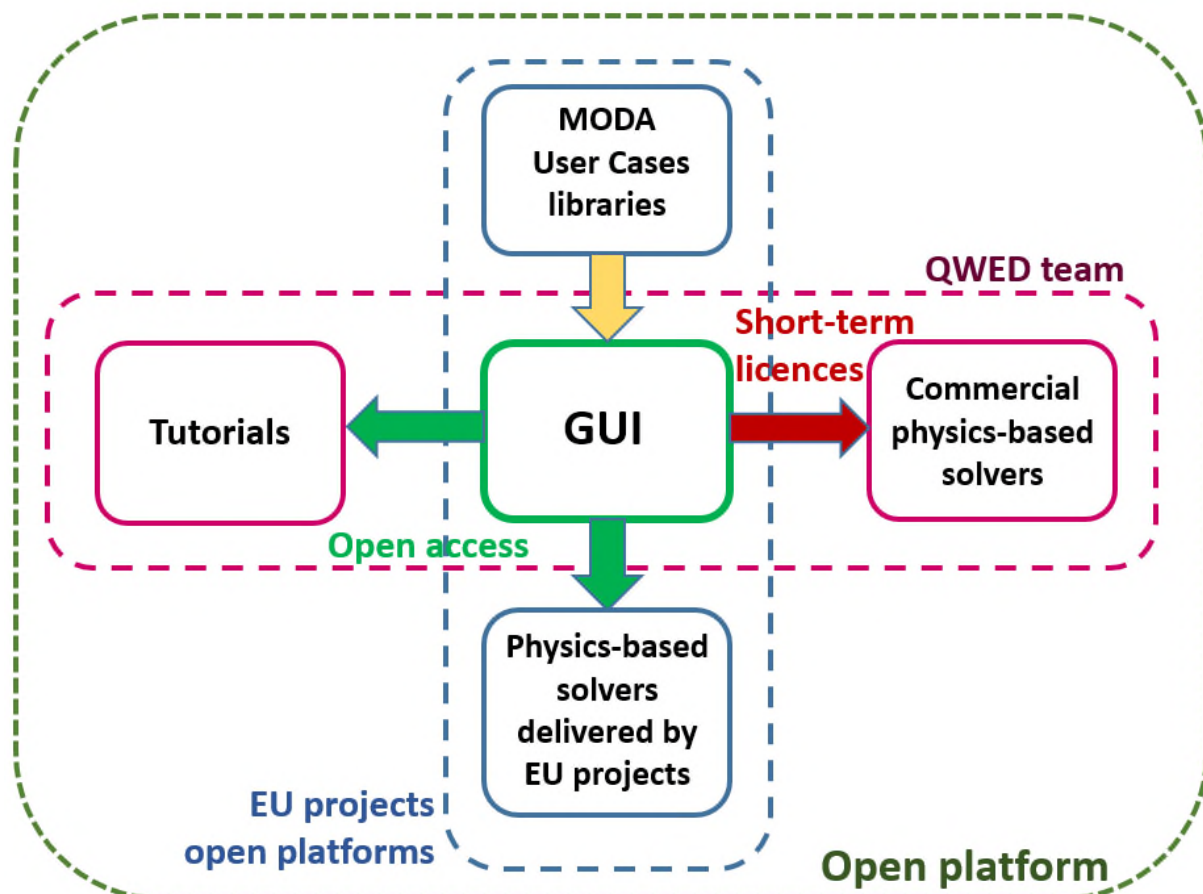

Fig. 20: The generalised concept of Open Platform - originating from the current MMAMA tools and examples.

3   CONCLUSIONS

In this Deliverable, the Open Platform has been set up. It contains a free-to-use parameterised GUI (MMAMA-Modeller), invoking representative FEM and FDTD solvers, of capabilities appropriate to the project dissemination and teaching purposes. The Open Platform includes examples of User Cases illustrating the physics of the material measurement scenarios investigated in the project, and necessary for extracting the material characteristics from measured data.

The proposed Platform is open not only in terms of access, but also of flexibility for further developments. It is assumed that further tools and examples will be added, by other research teams and projects. To facilitate such collaborations, the concept has been advocated in different communities:

- European Materials Modelling Council [14],
- computational electromagnetics [13].
- microwave engineering [15].

Dissemination will continue in the coming months on websites and social media:
info on QWED main webpage: https://www.qwed.eu/
MMAMA-Modeller installation's movie: https://www.qwed.eu/mmama_modeller.html
Facebook: https://www.facebook.com/QuickWave.QWED
LinkedIn: https://www.linkedin.com/company/qwed-sp-z-o-o-

To continue on the Open Platform developments, a *Task Group* on *Models Linking and Coupling (through Open Platform GUI)* has been proposed within the EMMC, to act on the interface of Model Development and Interoperability Focus Areas [2].

4 REFERENCES

[1] H2020 MMAMA project reports. [Online]. Available: www.mmama.eu

[2] The European Materials Modelling Council. [Online]. Available: https://emmc.eu/

[3] *What Makes a Material Function? - Modelling in H2020 NMBP Programme Material Projects,* Sixth Version, 2017, ed. Anne F. de Bass, Directorate-General for Research and Innovation Industrial Technologies. DOI: 10.2777/417118

[4] Smajic, J., How to Perform Electromagnetic Finite Element Analysis, Hamilton, UK: NAFEMS Ltd., 2016.

[5] QuickWave EM Software (1997-2020). [Online]. Available: https://www.qwed.eu/quickwave.html

[6] PathWave EM Design (EMPro) Software. [Online]. Available: https://www.keysight.com/zz/en/products/software/pathwave-design-software/pathwave-em-design-software.html

[7] Celuch, M., and W. Gwarek. "Accurate analysis of whispering gallery modes in dielectric resonators with BoR FDTD method." 2018 22nd International Microwave and Radar Conference (MIKON). IEEE, 2018; DOI: 10.23919/MIKON.2018.8405207; (accepted) https://www.qwed.eu/qwed_mikon_2018.pdf

[8] Gungor, A., M. Celuch, J. Smajic, M. Olszewska-Placha, J. Leuthold "Flexible Electromagnetic Modeling of SMM Setups with FE and FDTD Methods", IEEE MTT-S International Conference on Numerical Electromagnetic and Multiphysics Modeling and Optimization NEMO 2019, Cambridge, 29-31 May 2019; DOI: 10.1109/NEMO.2019.8853672 (accepted) https://www.qwed.eu/publications/NEMO_Cambridge2019_2_paper.pdf

[9] Gungor, A., J. Smajic, F. Moro, and J. Leuthold, "Time-domain coupled full Maxwell- and drift-diffusion-solver for simulating scanning microwave microscopy of semiconductors," Photonics & Electromagnetics Research Symposium PIERS 2019; https://zenodo.org/record/4010220#.X04HUcgzZPZ

[10] F. Kienberger, "Overview of Scanning Microwave Microscopy", slides. [Online]. Available https://www.mmama.eu/oip/SMM/Keysight_SMM_Overview_MMAMA_2019.pdf

[11] Gungor, A., M. Celuch, J. Smajic, M. Olszewska-Placha, J. Leuthold " Electromagnetic and semiconductor modeling of scanning microwave microscopy setups ", submitted, (revision process going on) for IEEE Journal on Multiscale and Multiphysics Computational Techniques, 2020.

[12] MMAMA Articles, Presentations & Posters by QWED. MMAMA Open Platform Tools & Examples. [Online]. Available: https://www.qwed.eu/mmama.html

[13] Olszewska-Placha, M., M. Celuch, T. Le Quang, A. Gungor, J. Hoffmann, J. Smajic, J. Rudnicki, "Open access CAD, EM tools, and examples for teaching microwaves", accepted for 23rd Intl. Conference on Microwaves, Radar and Wireless Communications MIKON-2020, Warsaw, 5-8 October 2020; https://www.qwed.eu/publications/MIKON_Warsaw2020_accepted_1.pdf

[14] Celuch, M., M. Olszewska-Placha, "Continuum modelling with QuickWave software – User Cases of MMAMA and NanoBat projects", eSSENCE-EMMC Meeting on "Multiscale modelling of materials and molecules - in complex systems", Uppsala, 8 June 2020 (virtual); DOI: 10.5281/zenodo.3906887.

[15] Celuch, M., M. Olszewska-Placha, J. Rudnicki, A. Gungor, J. Smajic, and J. Leuthold, "Open platform GUI for comparative FDTD and FEM computation of material microwave measurement scenarios", accepted to 19th Biennial IEEE Conf. on Electromagnetic Field Computation CEFC-2020, Pisa, originally scheduled April - postponed to 16-19 Nov. 2020; https://www.qwed.eu/publications/CEFC_Pisa2020_accepted.pdf