



WM-01

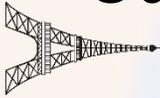
Advances in full-wave computational modelling of microwave probe – material interactions to support metrology applications

Dr. Malgorzata Celuch

QWED Sp. z o.o., Warsaw, Poland

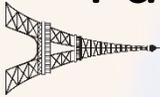
Email: mceluch@qwed.eu





- I. Introduction
- II. Full-Wave Electromagnetic (EM) Modelling
- III. Methodology
 - Conformal Finite-Difference Time-Domain (FDTD) Algorithms
 - Vector 2D Model of the Probe Region
- IV. Co-Processing Functions
- V. Results and Achievements
 - Ultra-Fast Computer Simulations
- VI. Case Studies and Applications
- VII. Conclusion

Full-Wave Electromagnetic (EM) Modelling

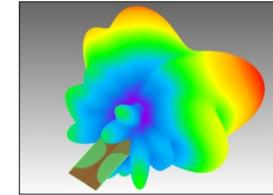


QuickWave

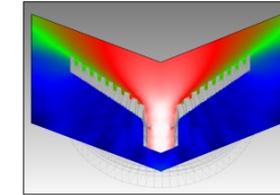
Software for electromagnetic design and simulations based on conformal FDTD method.

QuickWave is a general-purpose electromagnetic simulator based on the conformal FDTD method and supplemented with a range of unique models for curved boundaries, media interfaces, modal excitation, and parameter extraction. It has a well-established position on the world's market due to approaching specific, challenging problems specialists participation in the customer's projects as consultants). That kind of approach causes that QuickWave has a very broad variety of information which can be extracted from the simulations in a form of different pre-processings, co-processings and post-processings.

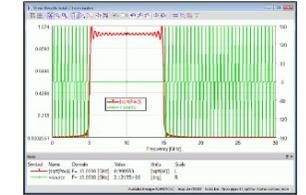
Functionalities



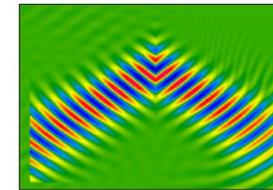
Full 3D EM solver



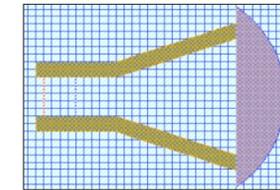
Vector 2D (V2D) solver for axisymmetrical structures (BOR - Bodies of Revolution)



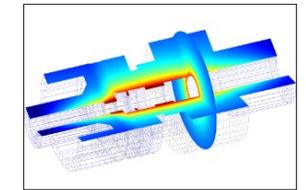
Co-processings & post-processings



Materials, excitations & boundary conditions

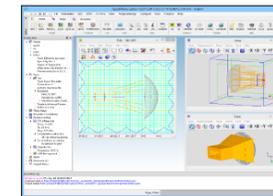


Conformal FDTD mesh

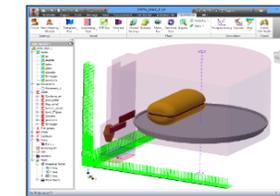


Special features

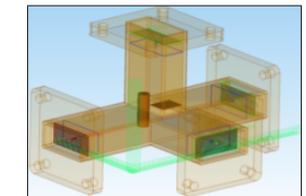
Input Interfaces



QW-Editor

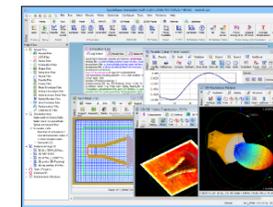


QW-AddIn for Autodesk® Inventor® Software

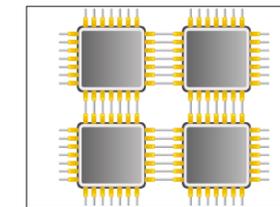


QW-Modeller

Simulation Engines



QW-Simulator

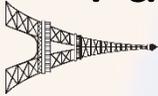


Multiprocessor / multicore computing



GPU / MultiGPU computing

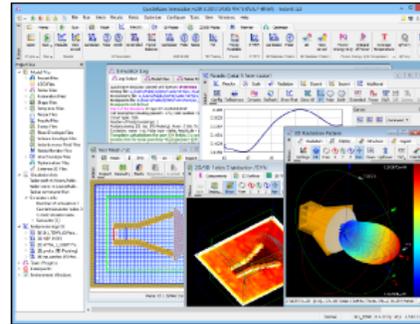
Full-Wave Electromagnetic (EM) Modelling



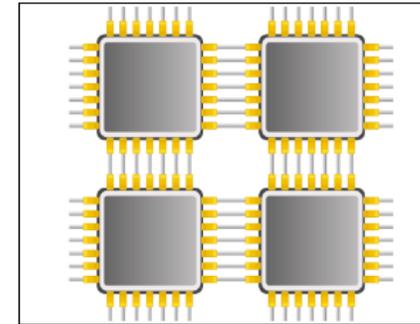
QuickWave Simulator (QW-Simulator) is the conformal FDTD simulation engine and conducts the FDTD calculations, extracts the desired frequency-domain parameters, displays all the computed fields and results, and allows saving them on disk.

QW-Simulator utilises state-of-the-art FDTD algorithms as well as many original models and procedures developed by the authors of the program during nearly two decades of intensive research on the time-domain electromagnetic modelling. These specialised features are well represented by the publications.

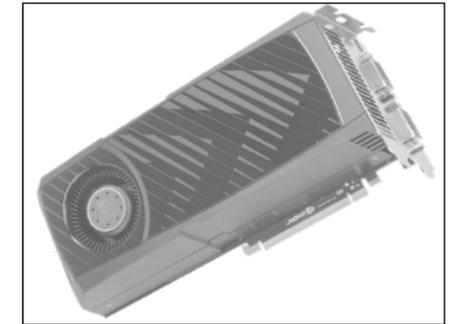
Simulation Engines



QW-Simulator

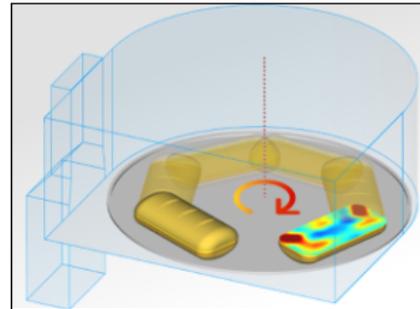


Multiprocessor / multicore computing

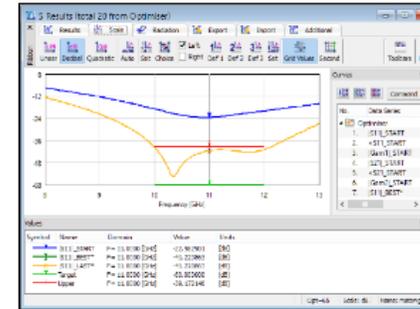


GPU / MultiGPU computing

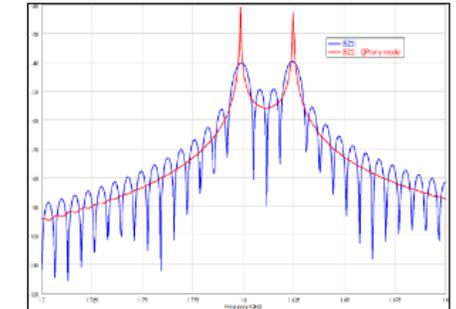
Specialised Modules



Basic Heating Module

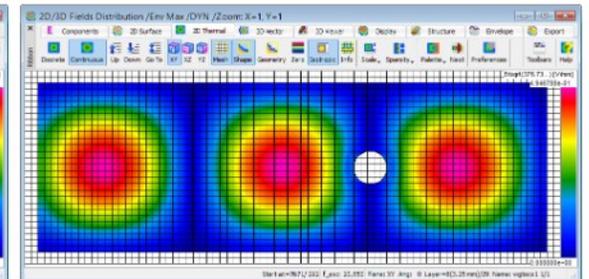
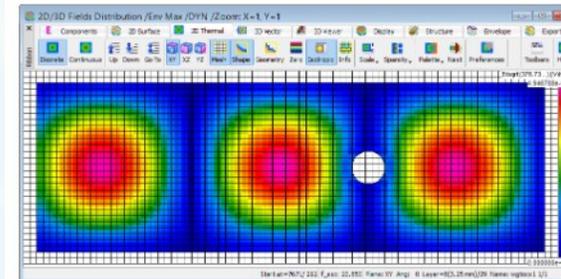
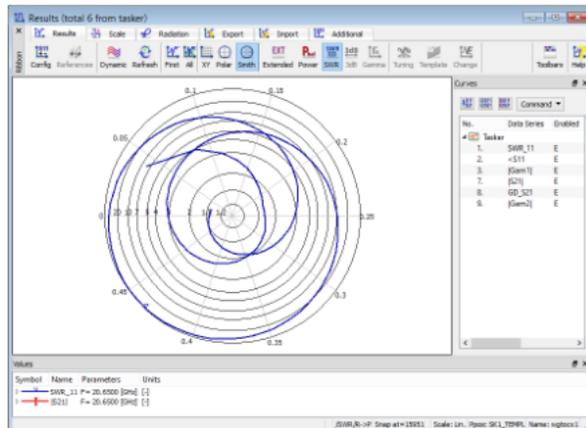
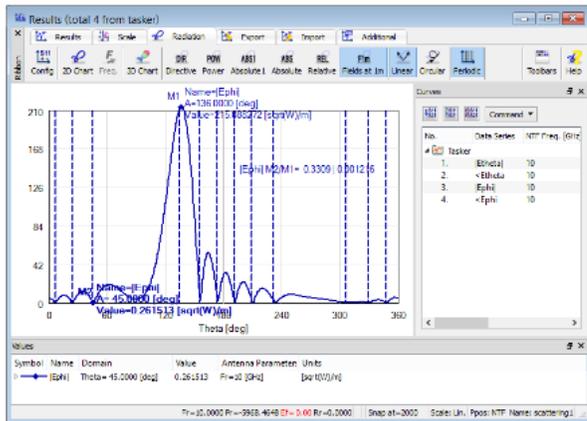
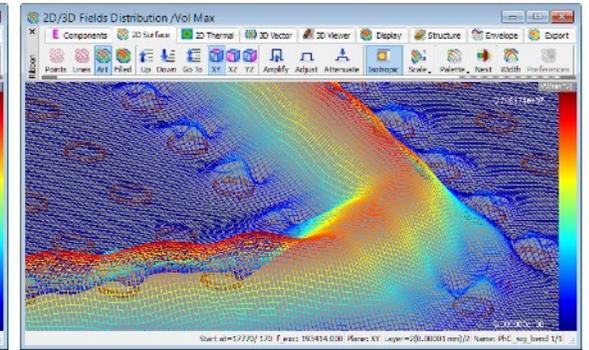
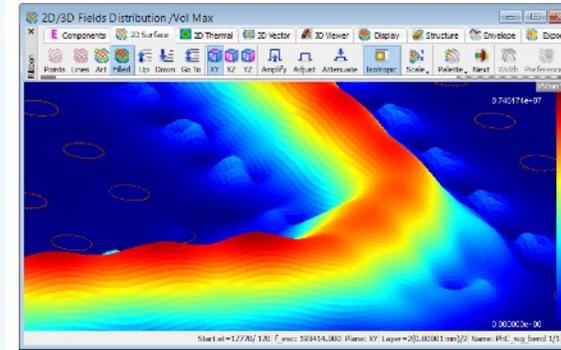
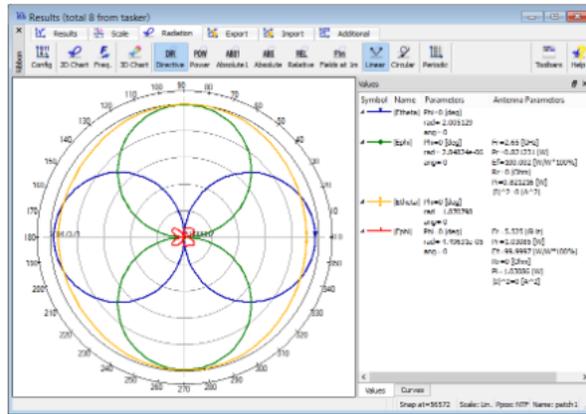
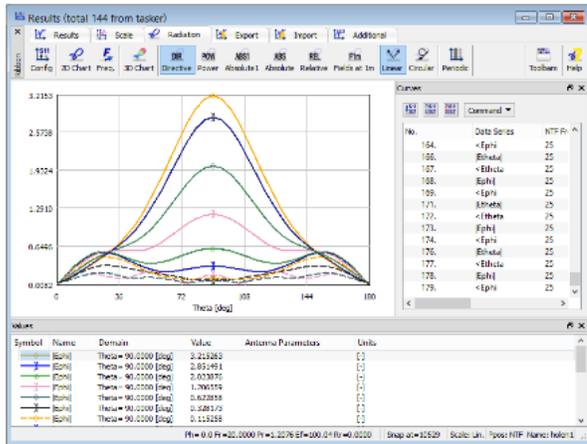
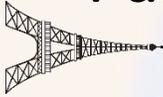


Multiobjective Optimiser

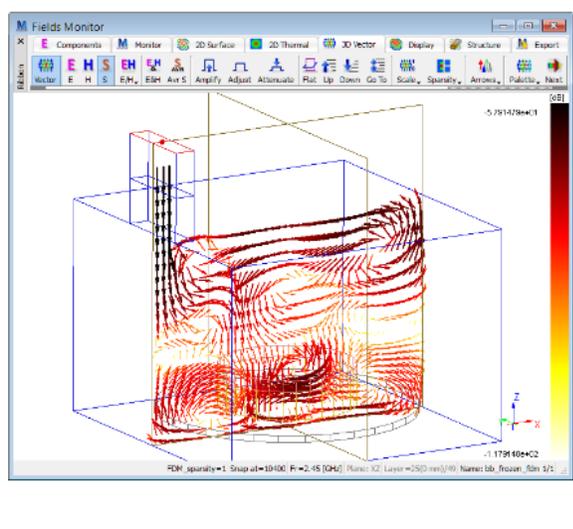
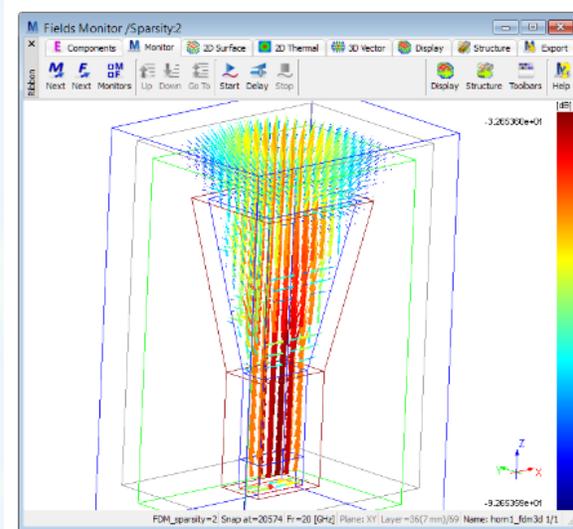
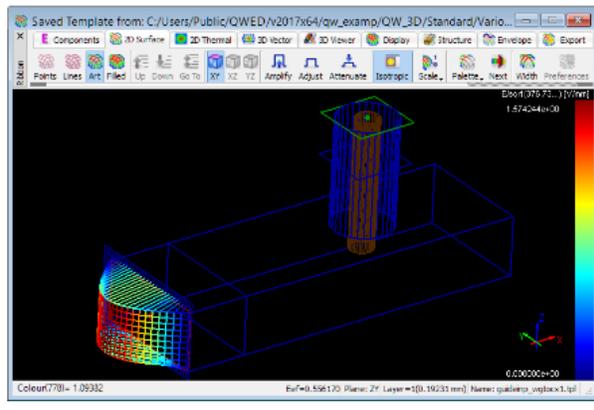
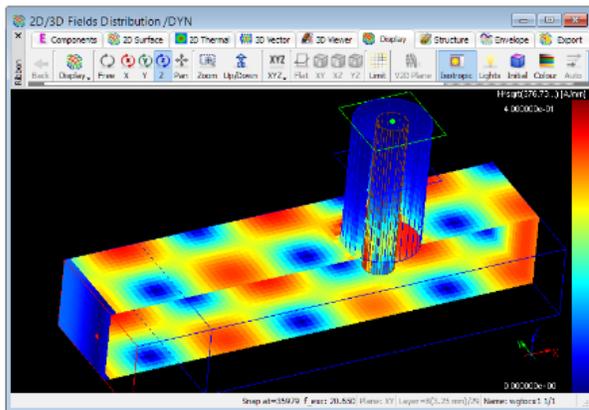
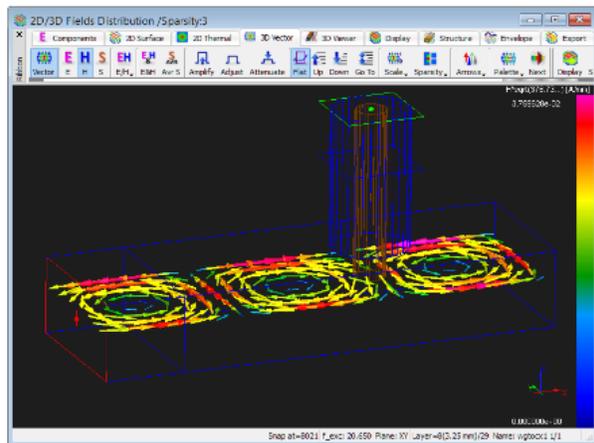
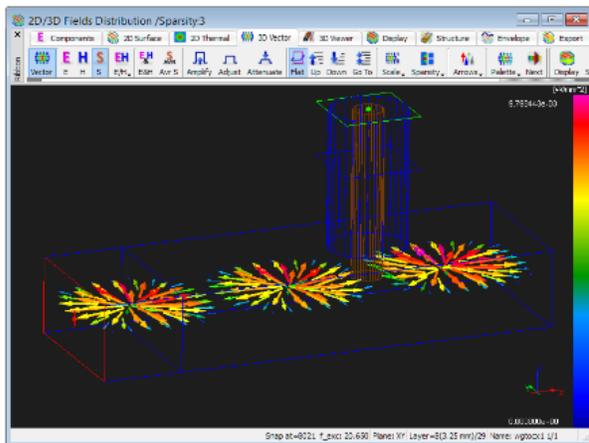
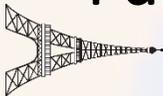


High Q structures analysis

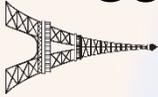
Full-Wave Electromagnetic (EM) Modelling



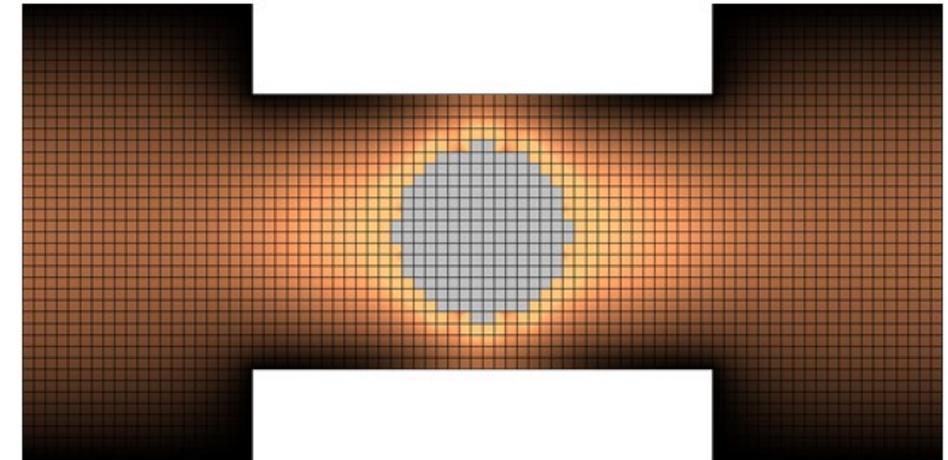
Full-Wave Electromagnetic (EM) Modelling



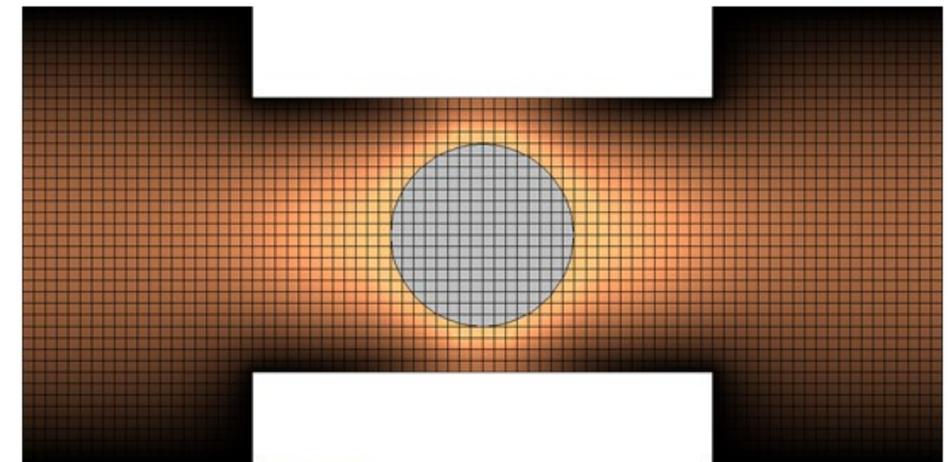
Conformal Finite-Difference Time-Domain (FDTD) Algorithms



Classically, in FDTD method the analysed circuit is divided into cuboidal cells, where each cell composes of only one medium. This type of meshing (dividing into cells) is called stair-case and is shown in Stair-case FDTD meshing example picture. Classical FDTD stair-case meshing radically corrupts the physical geometry. Good shape imitation can be approximated by mesh refinement, but it should be noted that it drastically increases memory occupancy and simulation time, e.g. decreasing the cell size in all three directions by 2, increases the memory occupation by a factor of 8, and the computing time 16 (!) times. There are various conformal FDTD techniques for better approximation of curved shapes, but they usually require time-step reduction (proportional to the smallest cell maintained) and hence longer simulation time. *QuickWave* uses original, advanced, and unique conformal FDTD formulation developed by the authors of the software. The FDTD method has been enhanced with conformal boundary models, which allow precise and accurate modelling of curved shapes and obtaining high accuracy simulation results **without time-step reduction**. The result of conformal FDTD meshing is shown in Conformal FDTD meshing in QuickWave picture. An improvement over classical FDTD is immediately visible. Let us emphasise that in both cases we are talking about an actual internal representation of the 3D geometry in the electromagnetic simulation process, and not about the graphical display shown by the geometry editor.



Stair-case FDTD meshing example.



Conformal FDTD meshing in *QuickWave*.

Vector 2D Model of the Probe Region

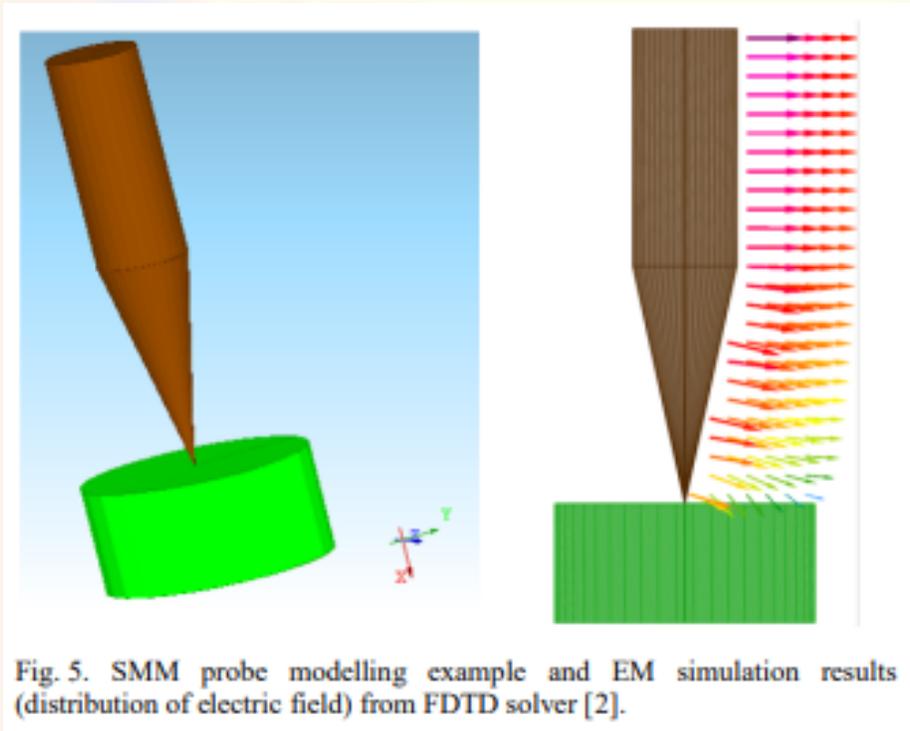
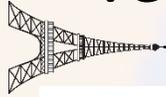


Fig. 5. SMM probe modelling example and EM simulation results (distribution of electric field) from FDTD solver [2].

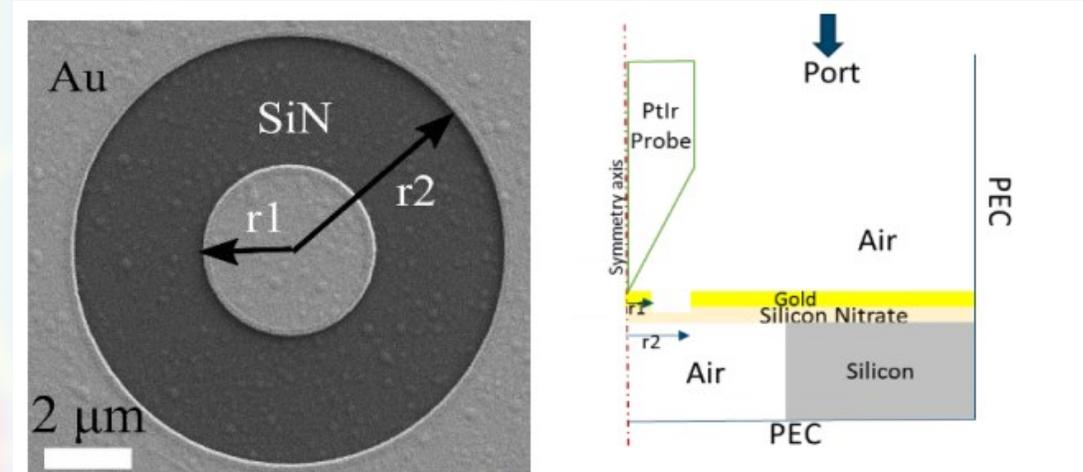
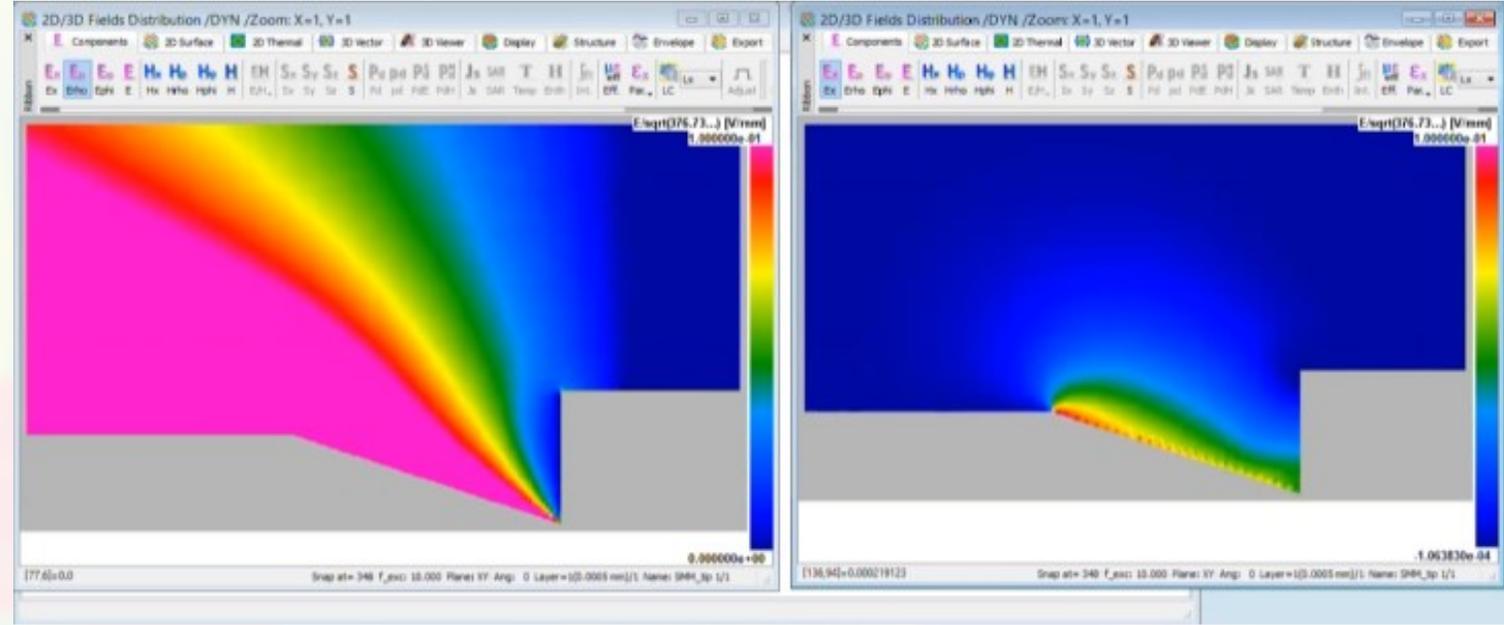
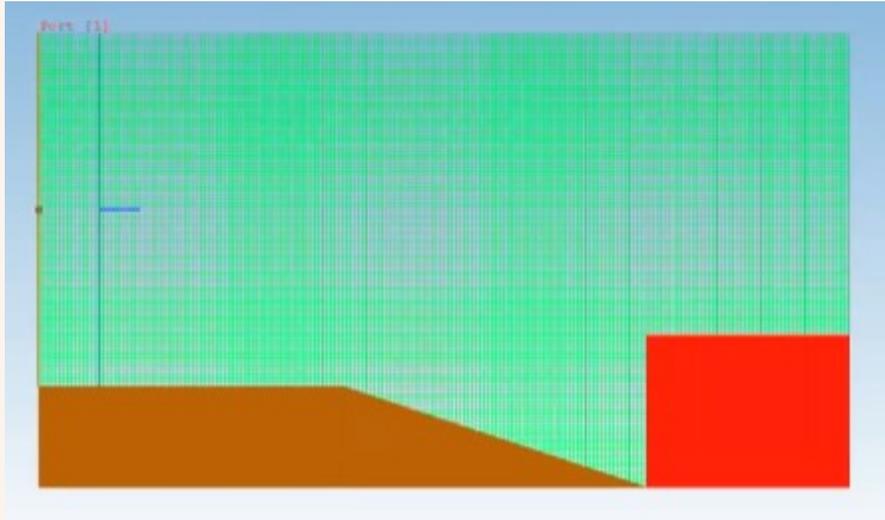
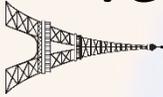


Fig. 6. Scenario for the extraction of capacitance of capacitors fabricated by METAS: a top view (SEM image) of one of the four fabricated devices (left) and simulation setup (right).

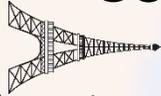
In simulations, the impedance is extracted by near-field integration close to the tip. Due to the locally quasi-TEM character (Fig. 5), E-field (voltage) integration is unambiguous while for H-field (current) a convention needs to be agreed, and circular contours at 30 μm from the tip are used. The arrangement of the columns in Table I is not coincidental: it emphasises that the calibrated measurements are in-between the results obtained from the FEM and FDTD models. This is consistent with the different convergence properties of FDTD and FEM, and illustrates the relevance of invoking different solvers from the same GUI, facilitating solver cross-comparisons and enhanced reliability of the model results.

Vector 2D Model of the Probe Region



User Cases relevant to SMM, dielectric resonator, and coaxial probe material measurements.

Co-Processing Functions



QuickWave is very flexible in so called co-processings. The user can open arbitrary number of windows for display of field components, dissipated power, Poynting vector etc. (in various graphical display systems and at any simulation stage). The decisions about the number and type of the windows showing valued deliverable form of the instantaneous filed components do not need to be taken prior to launching the simulation.

The co-processings data are available (for viewing, storing, etc.) at any simulation stage.

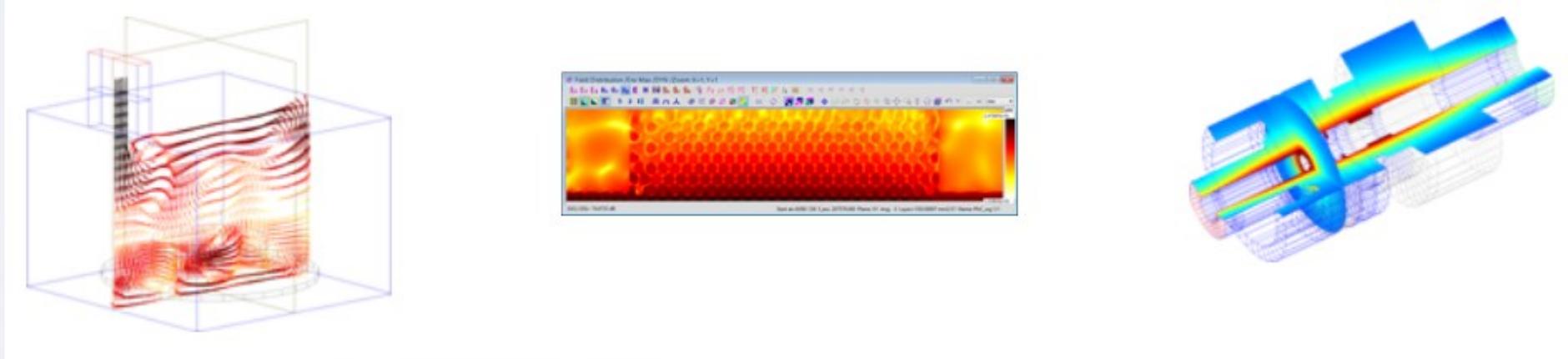
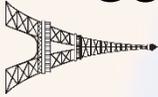
See complete description about co-processings.

Display:

- various display types for field distribution viewing (quasi-three-dimensional, fields intensity represented by colours, vector form)
- linear and decibel scales
- automatic and manual scales
- one and two dimensional displays
- two dimensional displays available for each cells layer
- 3D presentation of the antenna radiation pattern
- 3D presentation of the field components distribution, currents, material parameters etc. using QViewer module
- instantaneous and envelope (i.e. time-maximum and time-averaged) values of the displayed component

Data:

- fields (E and H field components), Poynting vector and power dissipated distribution available at any simulation stage (time domain monitoring)
- fields (E and H field components), Poynting vector and power dissipated distribution for real and imaginary grids, available for the periodic structures
- SAR calculations
- temperature and enthalpy distribution for microwave heating problems
- effective media parameters distribution
- watching field components along a specified line in space/versus time/along pre-defined contour
- virtual measurements of attenuation and SWR
- Time-Domain Reflectometry results (with virtual measurements of reflection coefficient and location of the discontinuity)
- power dissipated and energy stored in electric and magnetic field, and the resultant Q-factor calculations (also for real and imaginary grids for periodic structures)
- power dissipated and stored energy calculations for the entire lossy volume or in the specified objects
- energy dissipated over the entire duration of a pulse of limited duration (power dissipated integration in time)

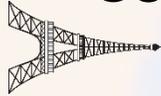


Here the tasks requiring calculation of the Fourier transformation of fields (S-parameters, radiation patterns or field distribution of a particular frequency extracted from pulse excitations) are included. In this case an apriori knowledge about the data to be accumulated during simulations is required (user chooses data that should be calculated before running the simulation).

All the post-processing data can be viewed, stored, etc., **at any simulation stage.**

Display

- ✓ linear, decibel, and quadratic (for S-parameters, radiation and scattering patterns) scales
- ✓ automatic and manual scales
- ✓ Smith and polar chart
- ✓ loading reference results for S-parameters, radiation and scattering patterns



S-parameters

broadband S-parameters extraction (results available at any simulation stage)

- full S-parameters matrix calculations (exciting the consecutive ports in sequential or multi-simulator regimes)
- -reciprocity option available for S-parameters calculation
- reflection coefficient calculations for several ports simultaneously, during a single simulation run (applicable for multi-source networks when N sources operate - simultaneously, and consequently the S-matrix cannot be calculated)
- virtual shift of the reference plane the plane where the S-parameters extraction is performed)
- frequency dependent wave impedance (reference impedance for S-parameters calculations) and propagation coefficient of transmission lines
- power balance calculation
- standing wave ratio (SWR) and group delay calculations
- S-parameters embedding and deembedding

Radiation and scattering

- antenna radiation patterns and scattering patterns of a scattering structures for wide angle range, at multiple frequencies, for any plane
- gain (directive, power, absolute, relative, fields scaled to 1m), radiation efficiency, radiation resistance and radiated power calculations
- radiation patterns for linear and circular polarisation
- radiation patterns for antenna arrays
- radiation pattern at a chosen near-to-far transformation (Huygens) surface
- far field 3D radiation patterns calculations
- radiation pattern calculations in an arbitrary isotropic medium
- radiation patterns for a specified directions versus frequency
- impulse response in the far-field

Co-Processing Functions



Lumped

Fourier transforms of terminal voltage across/current through resistor at any circuit point

Fourier transforms of field integrals along defined contours

power available from the source calculations (Fourier transform of the excitation waveform)

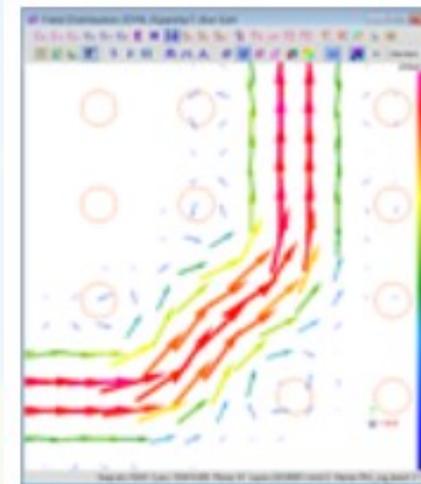
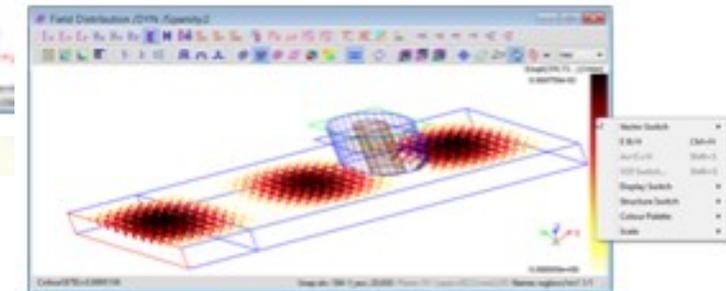
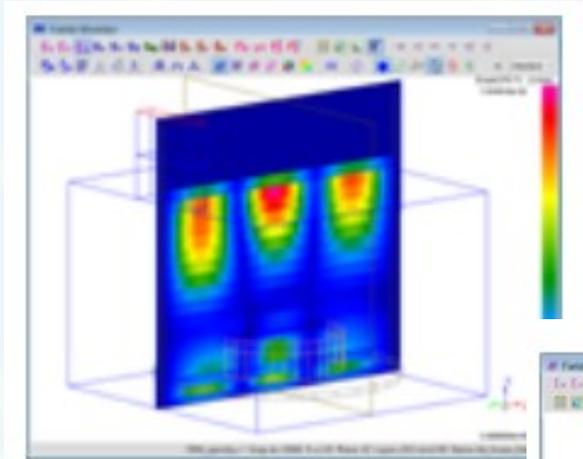
energy available from the source

Fields

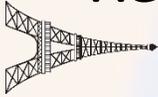
monitoring the field distribution at multiple frequencies in one simulation (frequency domain monitoring) with a sparsity factor in space and time

animation of the time domain field distribution (at chosen frequencies) for frequency domain monitoring

time integration of the Poynting vector



Results and Achievements



Conformal BoR FDTD modelling *Let's start designing*

The most popular variant is 3D FDTD in Cartesian coordinates, but for structures preserving the axial symmetry of boundary conditions another FDTD variant, namely the **Bodies-of-Revolution (BoR) FDTD** is advantageous. It incorporates the angular field dependence (angular mode number) analytically and restricts the spatial discretisation to half of the longitudinal long-section of the antenna. It has been broadly used for corrugated horns and now tested for the multiflare horn herein. In contrast to the fixed rectangular grid used in the FDTD method, conformal FDTD makes the computational domain consistent with the boundary of the object being modeled. This approach allows for more accurate modeling of objects with curved surfaces and complex shapes, making it a valuable tool in a variety of applications.

	Diameters [mm]				Lengths [mm]		
Symbol	D_1	D_2	D_{sp}	L_1	L_2	L_3	
Value	0.406	0.976	1.19	2.4	0.487	0.398	7.886

Dimensions of the modeled antenna

NanoBat Modeller
licence-free CAD modeller developed within the NanoBat project.

Simulation parameters

Source is excited by Circular TE_{11} field mode at matching frequency equal **700 GHz**.

Setting up the source

Create a mesh

3D view of the considered multiflare antenna in NanoBat Modeller, which automatically generates 2D BoR mesh.

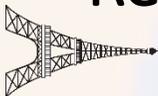
Getting results

The mesh is imported into the **BoR FDTD** NanoBat software and as one of the results of such a simulation, we get the return loss.

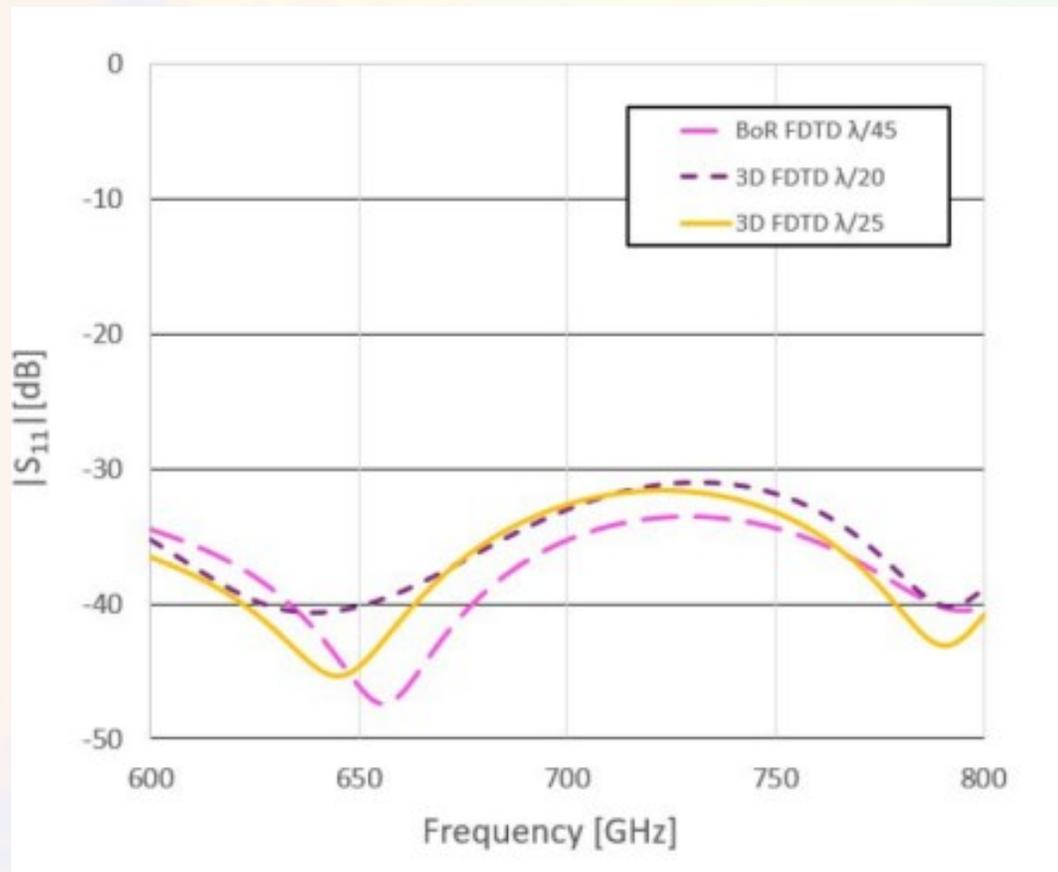
Return loss calculated by **BoR FDTD** at meshing of $\lambda/30$ (CPU time 3 seconds) and $\lambda/45$ (10 seconds).

Electric Field distribution

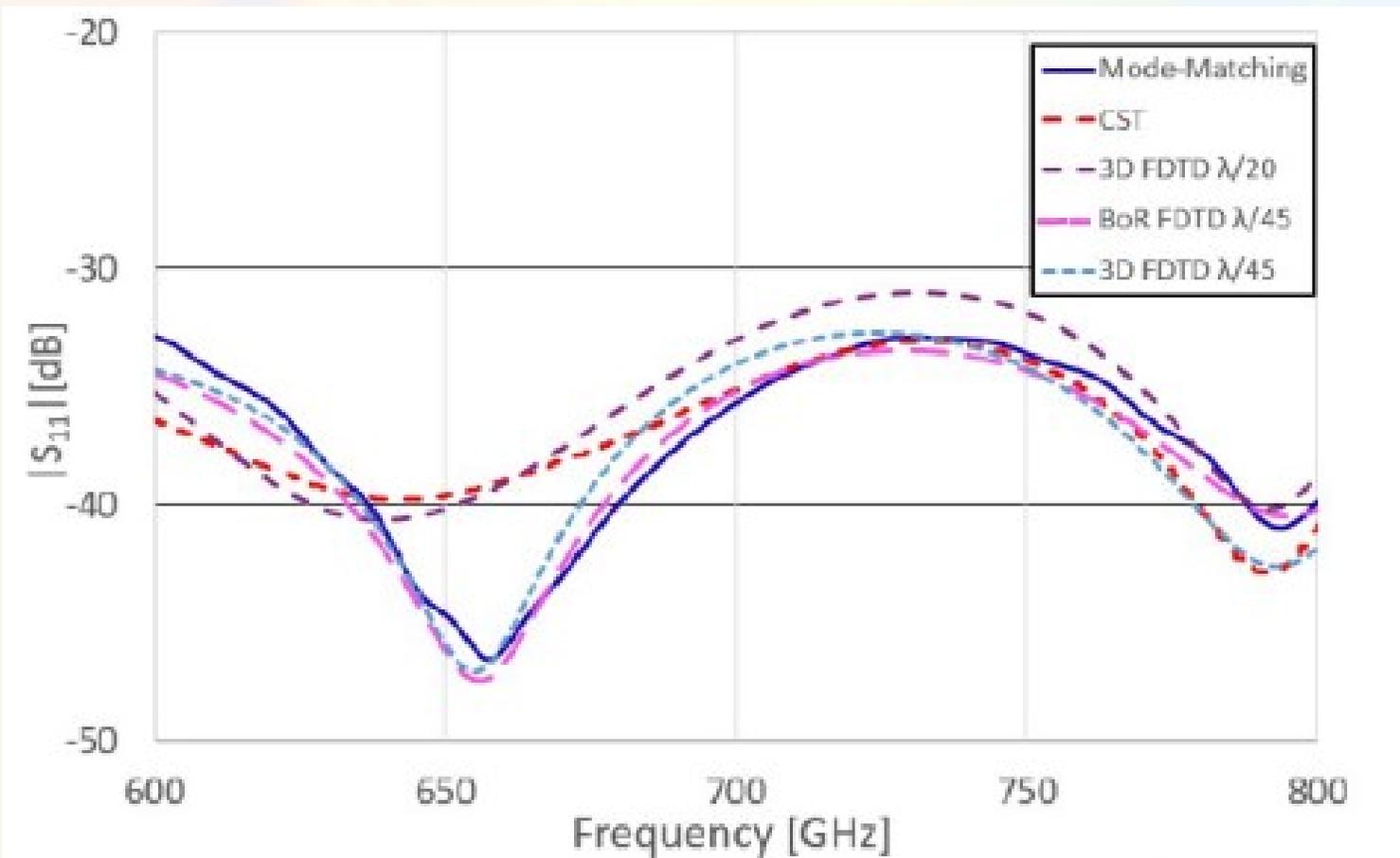
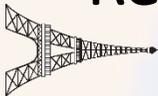
A commercial tool was used to illustrate the fields.



3D FDTD vs BoR FDTD

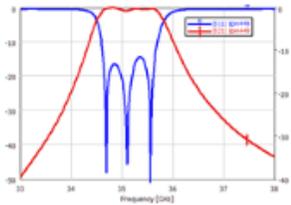
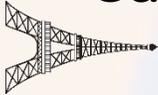


When considering **3D FDTD** calculations from 31 MB of RAM, as much as 4 GB should be allocated if $\lambda / 20$ resolution is set, which is equivalent to 50789508 cells. Increasing the resolution to $\lambda / 25$ results in an increase in the order of an additional 4 GB of memory. However, it can be seen that as the resolution increases, the results of the S11 scattering matrix approach the **BoR FDTD** solution which is shown above on Fig.3. The increased amount of resources is associated with an increase in calculation time to 02:07:45 hours for $\lambda / 20$ and 2:48:17 hours for $\lambda / 25$. With higher resolution Both **3D FDTD** and **BoR FDTD** methods were performed on a standard computer with parameters: i7-8700, 16 GB RAM and AMD Radeon Pro WX 3100. A change of computer was required to get results for **3D FDTD** with the $\lambda / 45$ resolution. This was needed because the 3D mesh uses a huge amount of RAM equal to 45.856 GB. Calculation time tooks 11:59:41 hours.



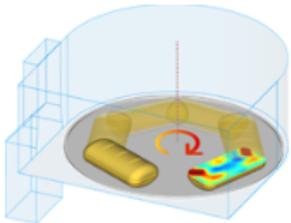
Benchmarking

For the **Mode-Matching** method, 140 mods are considered for this type of antennas, where the number of modes at each discontinuity is assigned in terms of the surface ratio between such discontinuity and the aperture. With this method, the calculations were completed in 686.1 seconds on the computer i7-4790 CPU and 31.8 GB RAM. All methods were compared to the commercial **CST** solution on figure below.



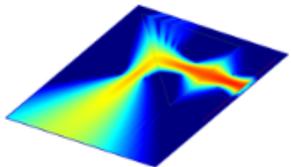
S-Parameters Extraction

S-Parameters extraction, including Sk1 parameters for reciprocal circuits and full S-matrix calculations, S-Parameters extraction below cutoff frequency, frequency dependent wave impedance, propagation constant, standing wave ratio and group delay, power balance calculations, S-Parameters extraction for virtually shifted reference (calculation) plane, etc.



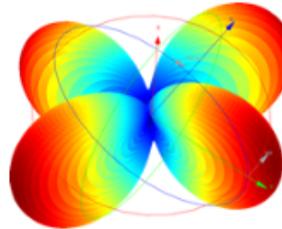
Microwave Heating

Microwave heating analysis, including loads rotation and movement along user defined trajectory, source frequency tuning to meet application specific requirements (e.g. maximising matching in microwave power applications with solid state power sources), source parameters switching, heat transfer analysis, and material parameters modification as a function of dissipated power.



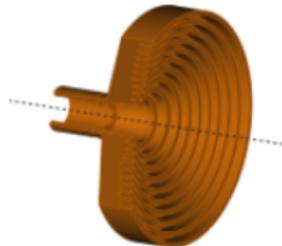
Materials

Analysis of wide variety materials, including isotropic and anisotropic dielectrics, single-, dual- and triple-pole dispersive materials including cold plasma, dispersive anisotropic dielectric given by Debye dispersion model, dispersive dielectric with third-order nonlinear polarisation, metamaterials (negative index materials, left-handed materials), temperature dependent materials (in Basic Heating Module), lossy metals (wideband modelling of skin effect), etc.



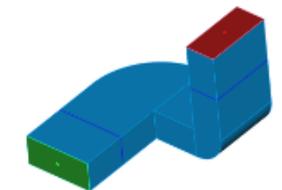
Radiation and Scattering Problems

Radiation and scattering patterns calculations, in a form of 2D and 3D characteristics, including radiation parameters extraction, e.g. antenna gain, power radiated, radiation efficiency, axial ratio, etc., extraction of linear and circular polarisation components, calculation of radiation and scattering patterns in an arbitrary isotropic medium, etc.



Bodies of Revolution

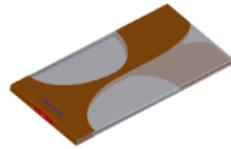
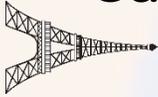
Ultra-fast vector 2D Bessel and FDTD hybrid solver (V2D BOR) designated for analysis of axisymmetrical Bodies of Revolution (BOR) structures.



Waveguides

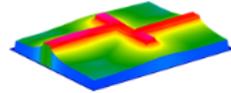
Rectangular and circular waveguide analysis, including inhomogeneous waveguides, transitions, bends, junctions, couplers, and waveguide resonators and filters.

Case Studies and Applications



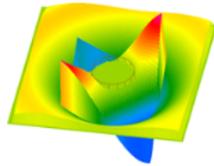
Planar Structures

Planar structures analysis, enabling application of infinitely thin metal layers (metal layers of zero thickness), including modelling of planar antennas, filters, couplers, etc.



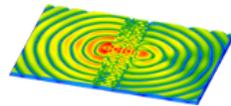
Filters

Analysis of planar and waveguide filters, including comb-line filters and dielectric resonator filters modelling also using QProny module for high Q structures.



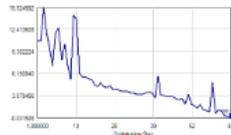
Free Space Incident Wave

Illumination with a free space incident wave, by a plane wave and 2D and 3D Gaussian beams, enabled also within dielectric and magnetic media and for periodic circuits.



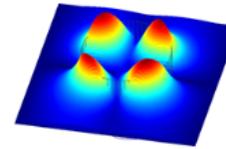
Photonic Crystals

Analysis of photonic crystals devices, including photonic crystal waveguide, waveguide bend, lens, etc.



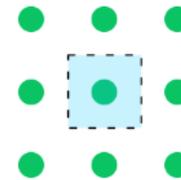
Optimisation

Multiobjective optimisation with QW-OptimiserPlus module.



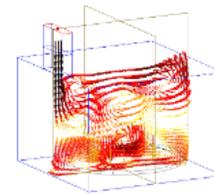
Resonators

Analysis of resonant structures, including waveguide resonators, dielectric resonators.



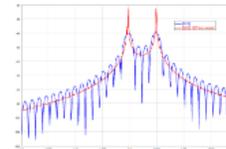
Periodic Structures

Analysis of infinite periodic structures using periodic boundary conditions (PBC), including analysis of eigenvalue problems, reflection characteristics of frequency selective surfaces (FSS), scatterometry of periodic structures, etc.



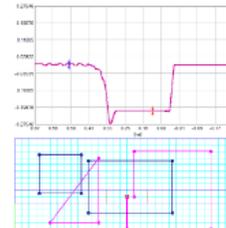
Frequency Domain Monitoring

Field distribution at selected frequencies from a time domain simulation with a pulse excitation.



High Q Structures

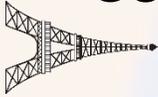
Analysis of high quality factor structures with specialised QProny module, enhancing the computation speed.



Time Domain Reflectometry and Field Integration Along Contours

TDR enabled by time domain signal displays. Currents and voltages extraction by integrating H-fields along a virtual loop surrounding a conductor and E-fields along a virtual line connecting two conductors.

Conclusion



In this study, we presented a comprehensive analysis of full-wave electromagnetic (EM) modeling using advanced methodologies and cutting-edge simulation techniques. We employed Conformal Finite-Difference Time-Domain (FDTD) algorithms to ensure high precision and accuracy in our simulations. By incorporating a vector 2D model of the probe region, we achieved a detailed understanding of the EM interactions.

Our approach was further enhanced through the integration of co-processing functions, allowing for real-time data processing and improved computational efficiency. The results obtained from our ultra-fast computer simulations demonstrated significant advancements in the field, highlighting the robustness and reliability of our methods.

The case studies and applications discussed in this work underscore the practical implications and potential uses of our modeling techniques in various domains. These applications not only validate our methods but also showcase their versatility and effectiveness in solving complex EM problems.

In conclusion, the methodologies and results presented in this study pave the way for future research and development in full-wave EM modeling. Our findings contribute to the ongoing advancement of computational electromagnetics, offering valuable insights and tools for researchers and engineers in the field.



**EUROPEAN
MICROWAVE WEEK**
PORTE DE VERSAILLES
PARIS, FRANCE
22-27 SEPT. 2024
www.eumweek.com

Waves Connecting Europe

Thanks!

Email: molszewska@qwed.eu

