Seminar for the "Materials for Energy and Electronics" Group,
University of Kent, 4 November 2021 (remote)

- *an invitation to collaborations…*
- *why set up an SME when you are a Ph.D. student?...*

Coupling materials modelling & measurements to fields & waves modelling & simulations

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www.qwed.eu

IEEE Poland Section Women in Engineering AG
Vice-Chair

www.ieee.pl/wie

IEEE MTT-1

https://mtt.org/technical-committees/mtt-1-field-theory-and-computational-em-committee/

European Materials Modelling Council
Co-Chair Model Development

www.emmc.eu

CEN Workshop on Materials Characterisation

www.cen.eu/news/workshops/Pages/WS-2020-010.aspx

EU H2020 NanoBat project

www.nanobat.eu

other projects & associations:

International Microwave Power Institute

…

Outline

1. My research background & origins of QWED company

2. Modelling & simulations of electromagnetics & multiphysics effects in the continuum

3. Electromagnetic characterisation of materials & test-fixture design

4. Business & entrepreneurship aspects

5. Open Modelling Platform

6. Could we collaborate in these areas?

Electromagnetics & EM modelling

Electromagnetics (EM) = physics governed by Maxwell equations

Frequency ranges: DC – static (f=0), microwaves (MW) – ca. GHz range (cm to mm), mmWaves (e.g. 5G), light (nm)..

Electromagnetic modelling, Computational Electromagnetics (CEM)

= solving Maxwell equations with boundary & initial conditions subject to material constitutive relations

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}$$

$$\nabla \cdot \vec{D} = \rho$$

$$\nabla \cdot \vec{B} = 0$$

$$\nabla \cdot \vec{J} = -\frac{\partial \rho}{\partial t}$$

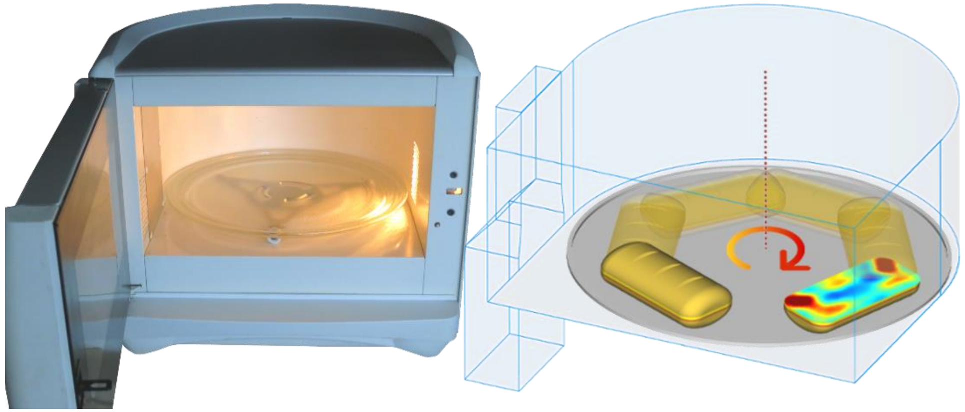
$$\oint_l \vec{E}\,\vec{\mathrm{d}l} = -\frac{\mathrm{d}}{\mathrm{d}t}\iint_S \vec{B}\cdot\vec{\mathrm{n}}\,\mathrm{d}s$$

$$\oint_l \vec{H}\,\vec{\mathrm{d}l} = \iint_S \left(\vec{J} + \frac{\partial \vec{D}}{\partial t}\right)\cdot\vec{\mathrm{n}}\,\mathrm{d}s$$

$$\oiint_S \vec{D}\cdot\vec{\mathrm{n}}\,\mathrm{d}s = \iiint_V \rho\,\mathrm{d}v$$

$$\oiint_S \vec{B}\cdot\vec{\mathrm{n}}\,\mathrm{d}s = 0$$

$$\oiint_S \vec{J}\cdot\vec{\mathrm{n}}\,\mathrm{d}s = -\iiint_V \frac{\partial \rho}{\partial t}\,\mathrm{d}v$$



general:

$$\vec{D}, \vec{B}, \vec{J} = F(\vec{E}, \vec{H})$$

typical:

$$\vec{D} = \underline{\underline{\varepsilon}} \cdot \vec{E}$$

$$\vec{B} = \underline{\underline{\mu}} \cdot \vec{H}$$

$$\vec{J} = \underline{\underline{\sigma}} \cdot \vec{E}$$

popular materials:

ε, μ, σ

scalar

(or diagonal tensors)

material parameters may also depend on: frequency, temperature, time, field strength,..

Two perspectives of EM modelling (continuum, physics-based)	
EM wave propagation in space (also in-between boundaries)	EM field interaction with materials
1990s: radars, radio & TV, electronic circuits	MW ovens
today: telecommunications (5G), RFID (ski-pass), IoT (wearable sensors)	biomedical (diagnostics – breast cancer, treatment – hyperthermia) MW chemistry, wood drying, plastics curing, rock comminution

"Modelling" for microwave technology: my *personal* view of history

Until 1980s:

- heuristic equations (experimental models; now fashionably called “data-based models”)
- lumped circuit approximations (0-dimensional: dimensions<< wavelength)
- 1D approximations (transmission lines, long lines, telegraphists equations, Smith chart)

In 1980-1990s:

- academic research on solving Maxwell eqs.

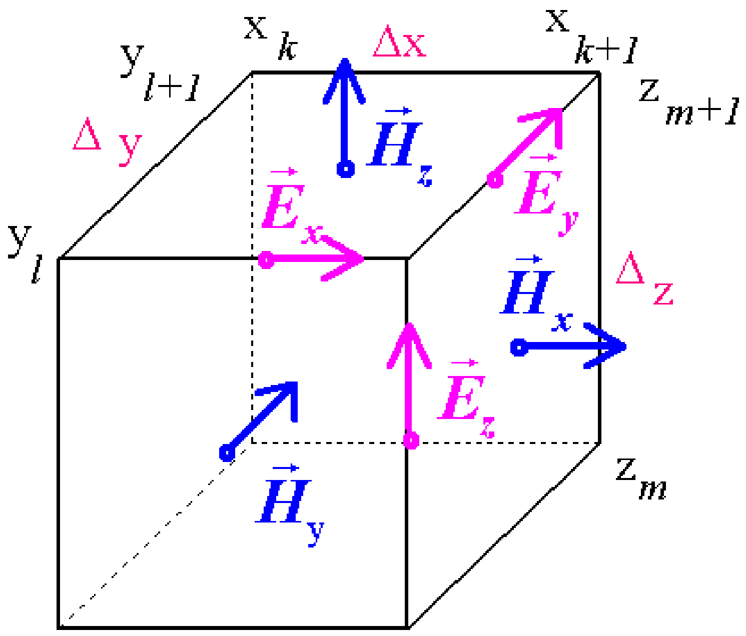
dimensionality in space	fields in space	fields in time
2D	modal expansions (method of moment, mode matching...)	monochromatic (frequency-domain)
3D	discretisation (FEM, **FD**, FV, TLM, SpN,..)	arbitrary (time-domain)

- commercial software packages implemented in industry
- **QWED follows FDTD approach based on original works of W.Gwarek & PhD work by M.Celuch**

Engineers question in 1990s: will EM software help me?
Engineers question today: can I trust EM software (to fully replace hardware prototyping)?

FDTD (Finite-Difference Time-Domain) for EM problems in 3D space

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \qquad \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$$



Yee cell, expanded node

Notation:

$${}_{k,l,m+0.5}E_z^{n} = E_z(x_k, y_l, z_m + 0.5\Delta z, t_0 + n\Delta t)$$

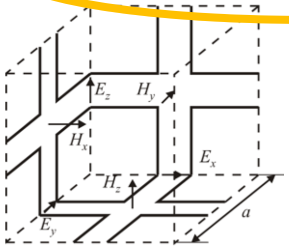
$${}_{k,l,m+0.5}E_z^{n+1} = E_z^{n} + \frac{\Delta t}{{}_{k,l,m+0.5}\varepsilon_z \varepsilon_0} \cdot$$

$$\cdot \left\{ \left[{}_{k+0.5,l,m+0.5}H_y^{n+0.5} - {}_{k-0.5,l,m+0.5}H_y^{n+0.5} \right] \frac{1}{\Delta x} + \left[{}_{k,l-0.5,m+0.5}H_x^{n+0.5} - {}_{k,l+0.5,m+0.5}H_x^{n+0.5} \right] \frac{1}{\Delta y} \right\}$$

Notes:

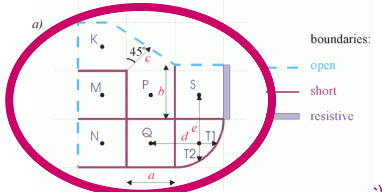
- E, H separated in time by half iteration (leap-frog)
- each field component defined at a different position in space

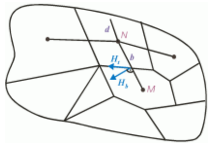
FDTD versus TLM
Theorem of Formal Equivalence



nodes: FDTD discretisation of Maxwell eqs.
connecting lines & stubs: TLM discretisation of Huygens principle

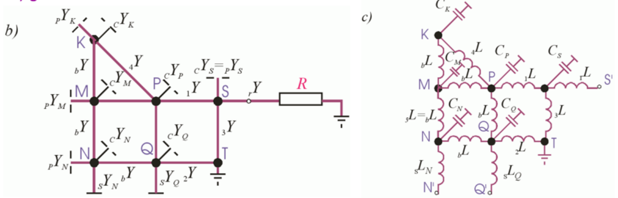
a) generalized gridding of a microwave structure

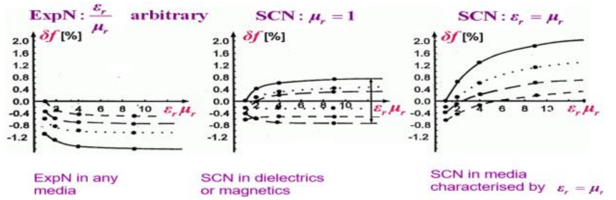


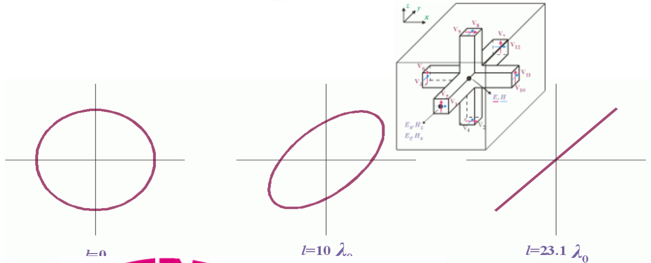


b) generalized TLM model

c) generalized FDTD model



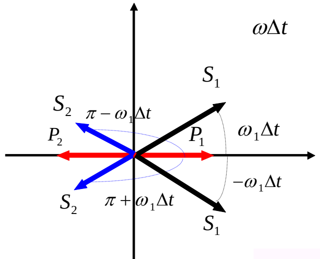


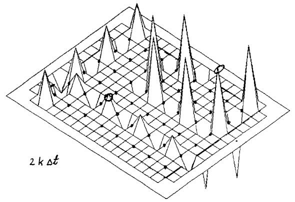


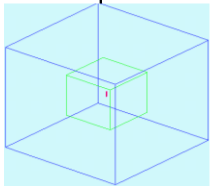
Generalised dispersion relations
Theory of P- and S-eigenmodes

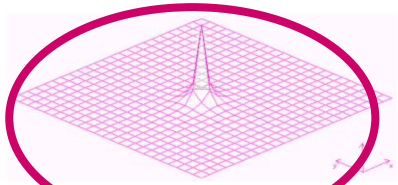
$$P(\omega\Delta t)\ \ S(\omega\Delta t,\ \beta_x a,\ \beta_y a,\ \beta_z a) = 0$$

$$\omega_{ph}^2[\,-\,\omega_{ph}^2\mu\varepsilon + \beta_{xph}^2 + \beta_{yph}^2 + \beta_{zph}^2]^2 = 0$$

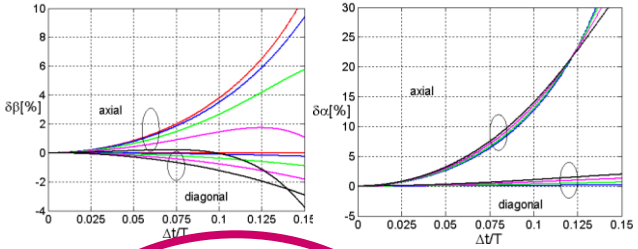




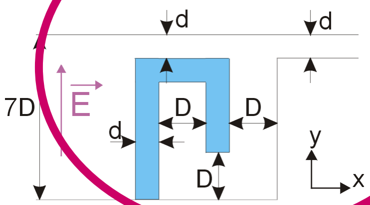


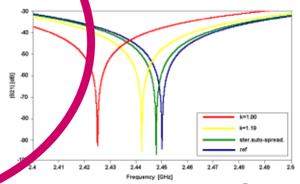


Dispersion in lossy media

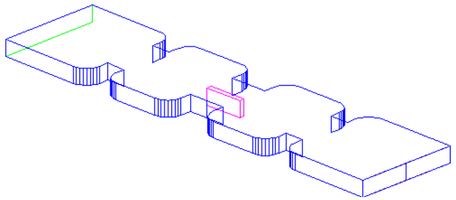


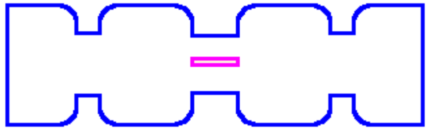
Field singularities

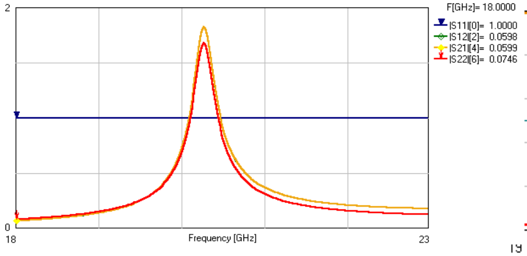


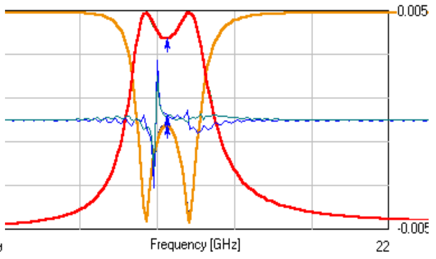


Generalised extraction of S-parameters in multi-modal transmission lines (incl. evanescent modes)

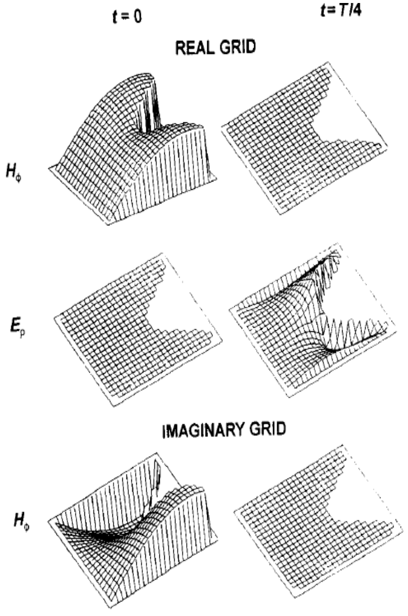




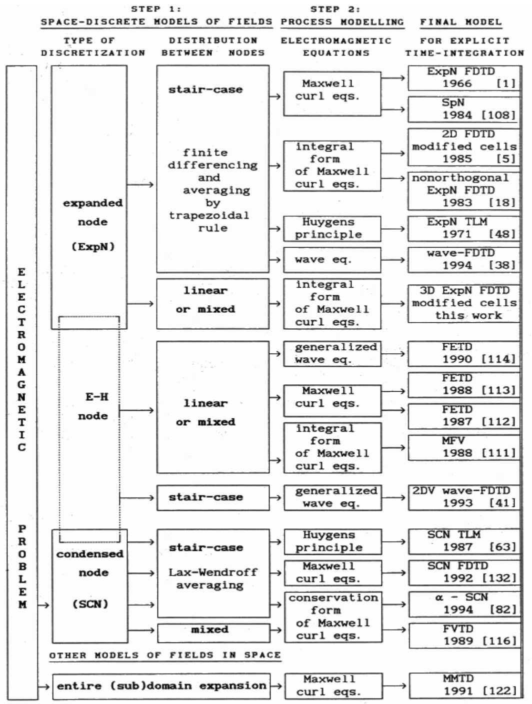




Periodic & vector 2D FDTD and TLM in real & complex form

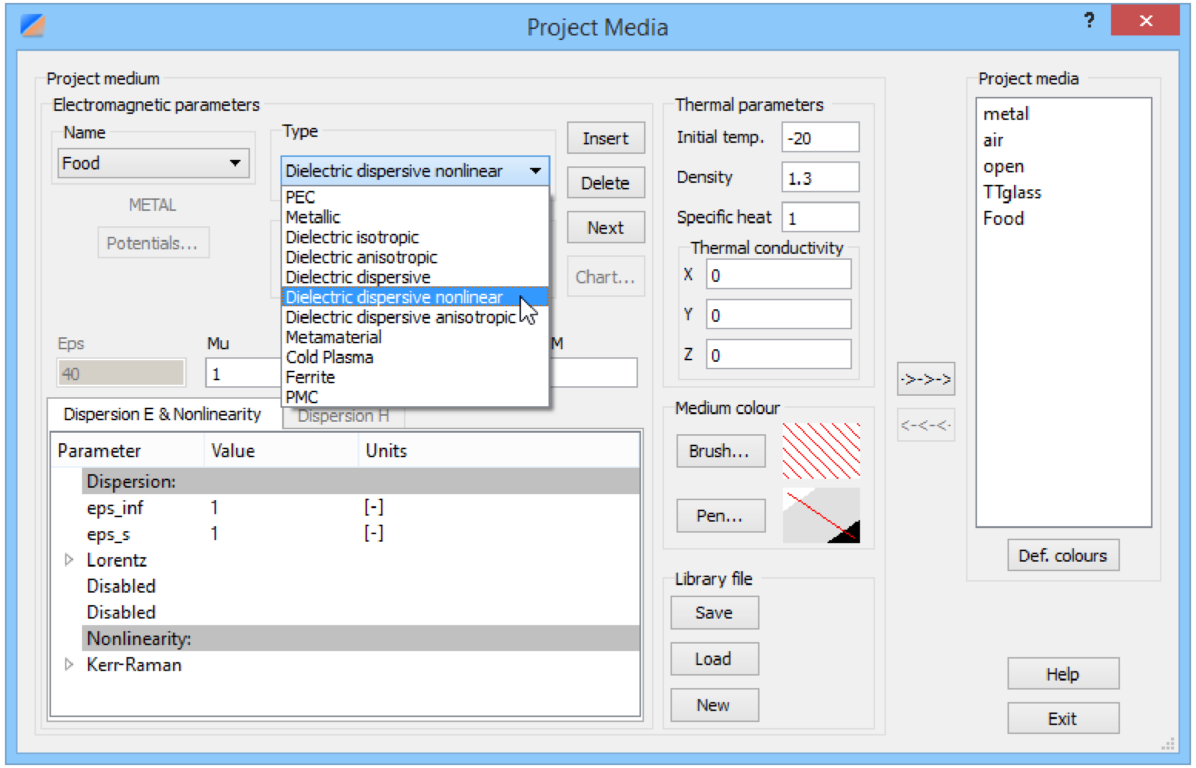


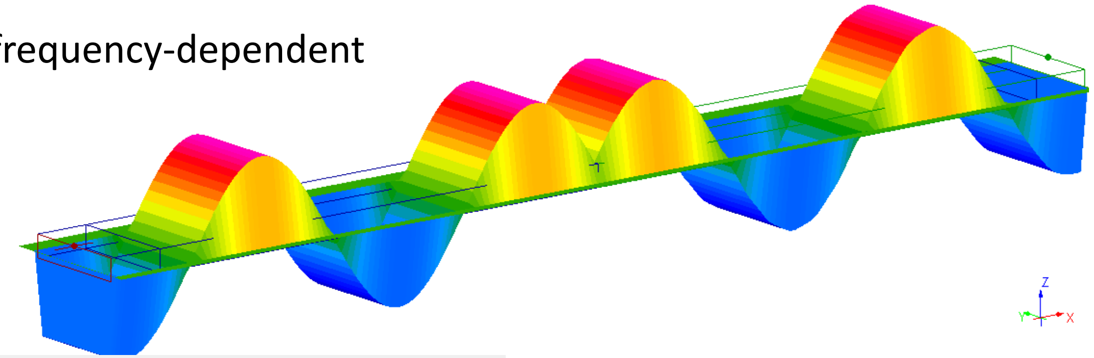
Classification of time-domain methods

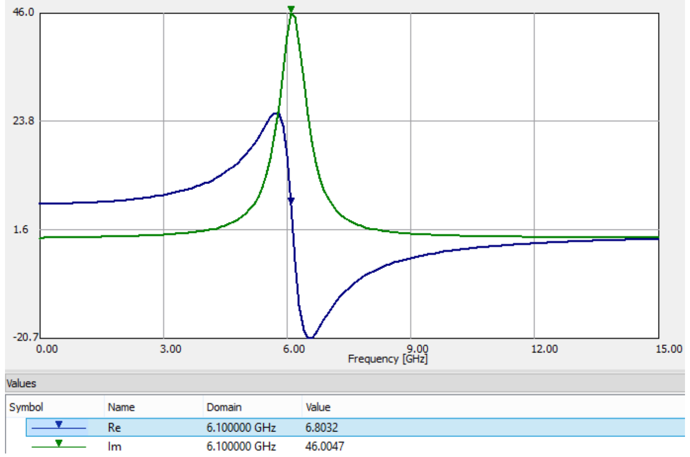


Material parameters in EM & multiphysics analysis

Various types of materials modelled by their macroscopic parameters – also frequency-dependent

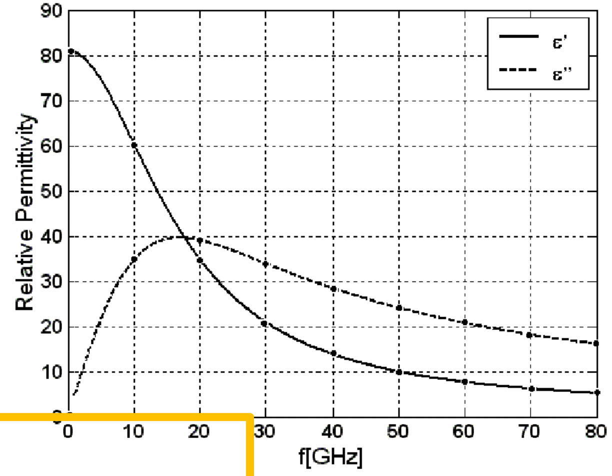






Lorentz model parameters from QuickWave™

Water parameters



Drude: $\varepsilon_r(\omega) = \varepsilon_\infty + \frac{(2\pi f_p)^2}{(j\omega 2\pi v_c - \omega^2)}$

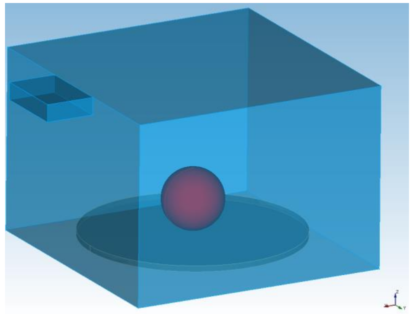
Debye: $\varepsilon_r(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{(1 + j\omega\tau)}$

Lorentz: $\varepsilon_r(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty (2\pi f_p)^2}{((2\pi f_p)^2 + j\omega 2\pi v_c - \omega^2)}$

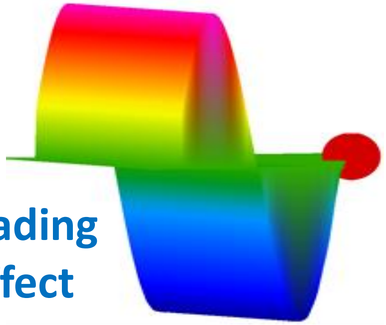
Material Libraries are key to EM software usefulness

Examples: EM field interaction with tissues

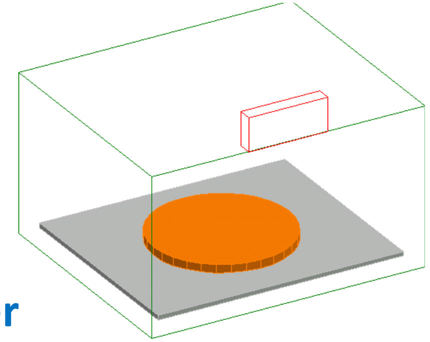
Separation of incident and diffracted fields (collaboration with *P.O.Risman, Malardalen Univesity*)



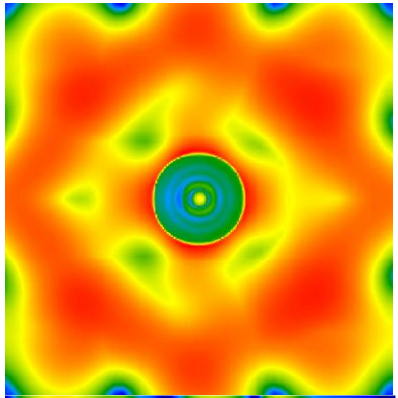
Exploding egg effect

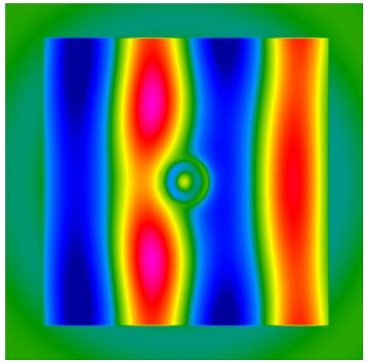


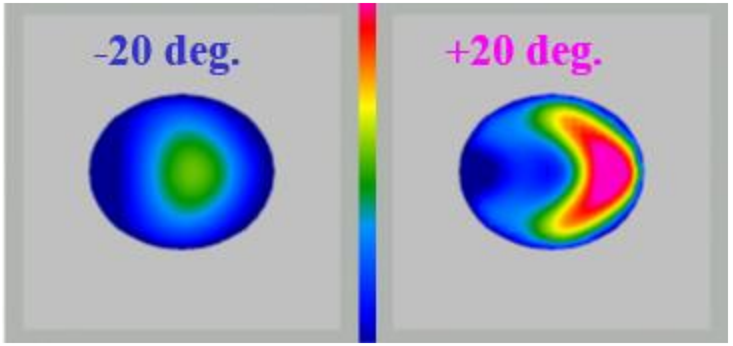
Heating beefburger



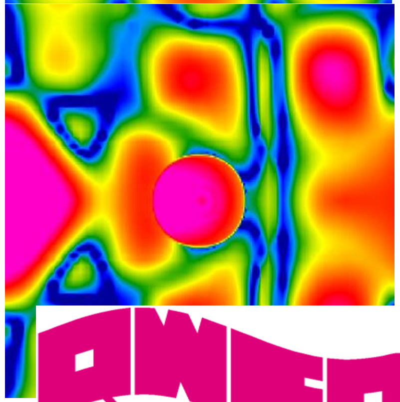
E-field

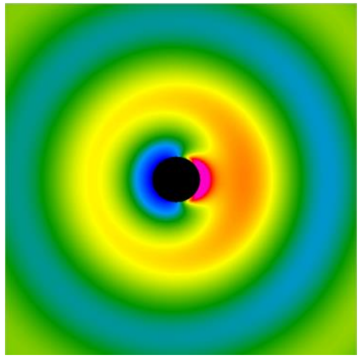


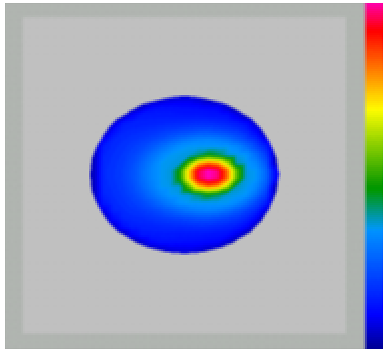




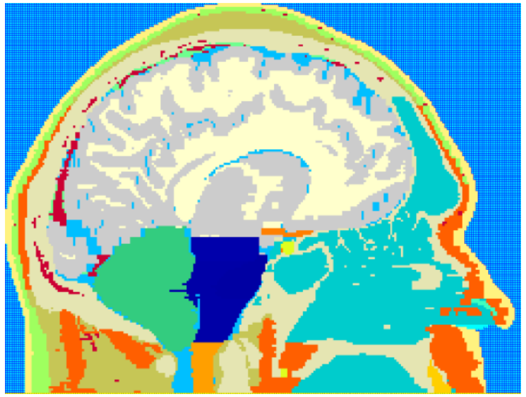
Scattered field



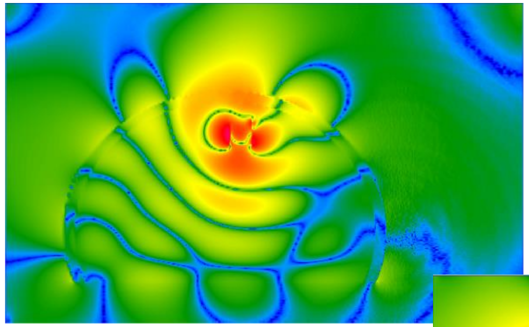


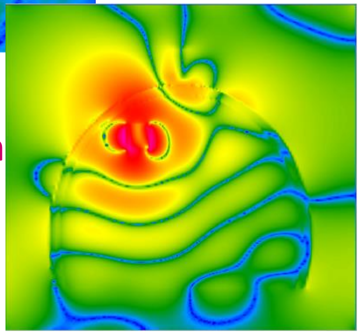


Detection of inhomogenities in tissues



AustinMan model* converted to **QuickWave EM** software for Mälardalen University, Sweden

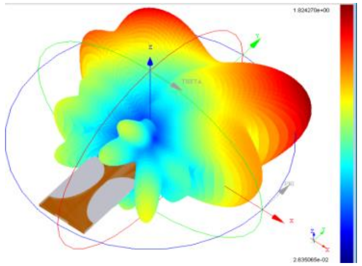




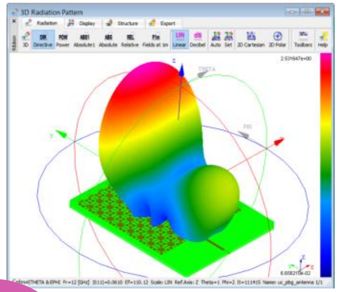
- ✓ **Tumours & haemorrhages detection**
- ✓ **Optimisation of multiantenna tomographic systems**

* https://sites.utexas.edu/austinmanaustinwomanmodels/

Examples: antenna systems with / for different materials

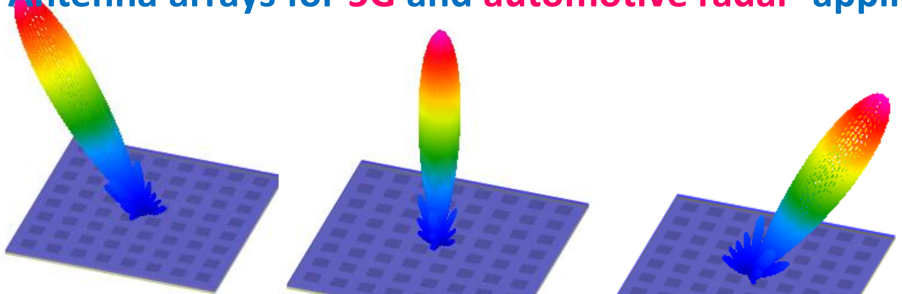


Balanced antipodal Vivaldi antenna & 3D radiation pattern at 10 GHz.

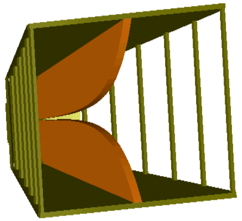


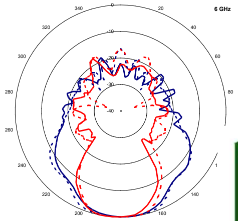
Aperture-coupled patch antenna on uniplanar photonic bandgap substrate & its radiation pattern at 12 GHz.

Antenna arrays for 5G and automotive radar application

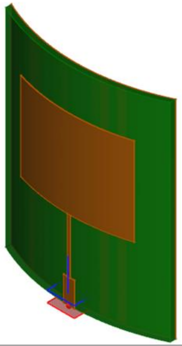


Designing and verifying tracking capabilities

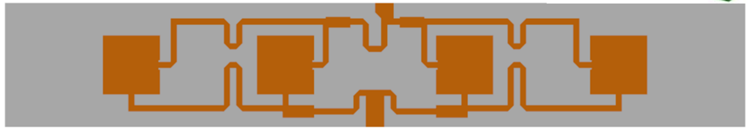




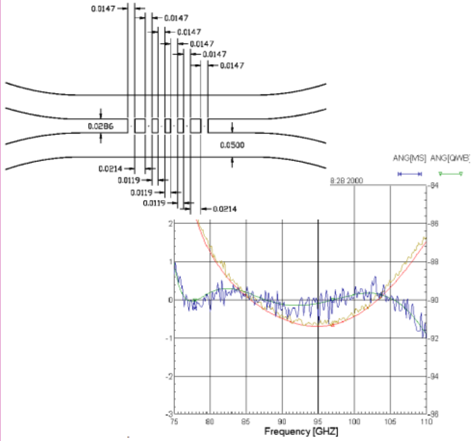
Pyramidal horn antenna for military surveillance measured (courtesy prof.B.Stec) & simulated patterns



Planar antennas for smart bio-sensors

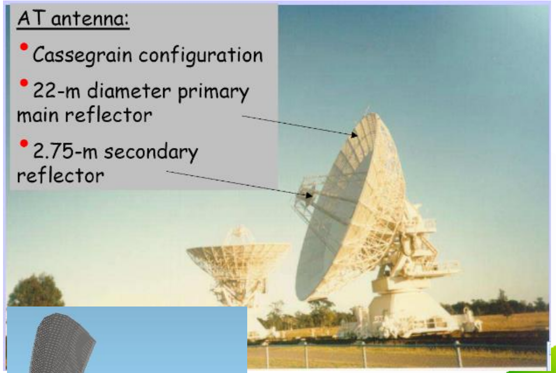


Antenna feed systems designed by NRAO



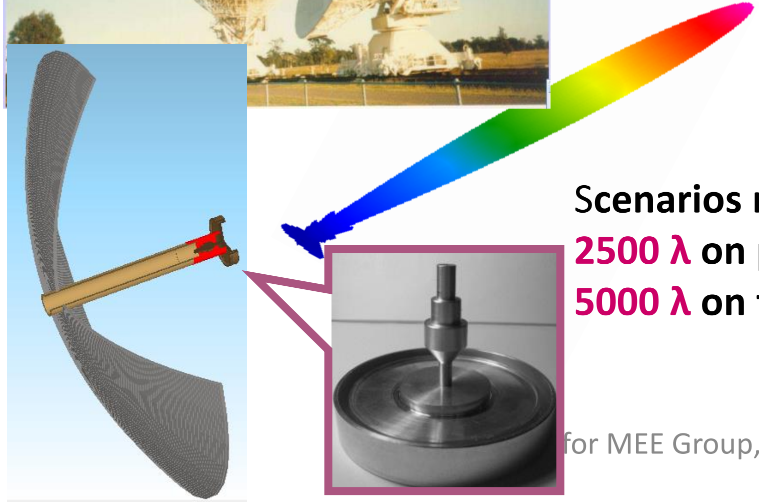
QuickWave 3D results at NRAO, see: ALMA Memos 381, 343, 325, 278.

Large dual reflector antennas: *Cassegrain, Gregorian, etc.*



BOR FDTD

Unique, ultra-fast vector 2D Bessel & FDTD hybrid solver for design & analysis of devices with axial symmetry

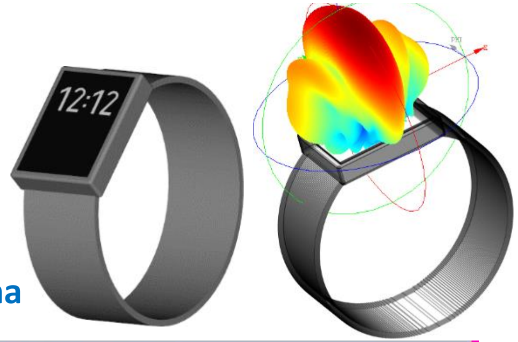


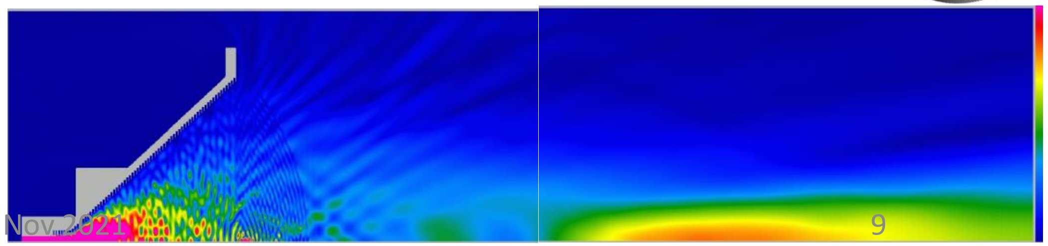
Scenarios modelled full-wave:

2500 λ on popular PC

5000 λ on top-shelf PC

Smartwatch with embedded patch antenna





Corrugated horn antenna for material measurements

Bilateral coupling of various processes - EM-thermal workflow

FDTD analysis with sinusoidal excitation at *f=f0*

Calculation of 3D pattern of ***dissipated power*** $P_{avg}(x,y,z)$

Enthalpy update in 3D domain

$$H^{n+1}(x,y,z) = H^{n}(x,y,z) + \frac{P^{n}_{avg}(x,y,z)\Delta\tau^{n}}{\Delta V(x,y,z)}$$

Temperature update in 3D domain
$T(x,y,z) = T[H(x,y,z)]$
from *.pmo file

Load movement/rotation
Translation of the object and thermal quantities along user-defined trajectory

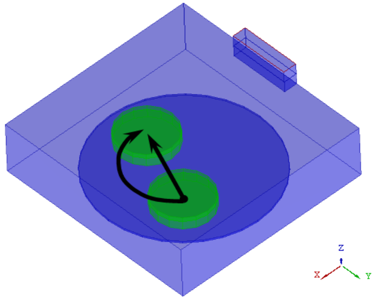
Calculation of heat transfer
Enthalpy and ***temperature*** update in 3D domain

Material and ***thermal parameters*** update in 3D domain $\varepsilon(x,y,z) = \varepsilon[T(x,y,z)]$
$\sigma(x,y,z) = \sigma[T(x,y,z)]$
from *.pmo file

Source tuning to *f=f1*
Changing operating frequency:
automatically to the deepest resonance or manually upon user's criterion

material parameters from user's text files (private data base)

```
#Raw beef draft media file for QW-BHM module (00-09-06 POR)
#Measurements & refinements by Per O Risman, Microtrans AB, Sweden
#Modified by QWED, Poland
# DATA FROM -20 C to +80 C, dH/dV in J/cm3 reversedEnth/Temp column
!Temperature    Enthalpy        EPa             SIGa    SpecHeat Density  Ka
# Data deg C    J/cm3                           S/m
-20             0               4.9             0.064   2.21     1.06     0.0069
-15             14.0            5.5             0.093   2.21     1.06     0.0069
-10             34.4            6.1             0.153   2.21     1.06     0.0069
-5              71.4            12.3            0.573   2.21     1.06     0.0069
-3              110.4           22.0            1.118   2.21     1.06     0.0069
-2.2            144.4           30              1.636   2.21     1.06     0.0069
-1.6            192.4           42              2.113   2.21     1.06     0.0069
-1.3            240.4           46              2.385   2.21     1.06     0.0069
-1.1            274.4           48.9            2.426   2.21     1.06     0.0069
-1.0            288.4           49.2            2.440   2.21     1.06     0.0069
10              327.9           48.9            2.317   2.21     1.06     0.0069
20              382.9           48.2            2.194   2.21     1.06     0.0069
35              450.4           46.9            2.072   2.21     1.06     0.0069
50              517.9           45.5            1.949   2.21     1.06     0.0069
65              585.4           43.6            1.922   2.21     1.06     0.0069
80              652.9           41.7            1.908   2.21     1.06     0.0069
```

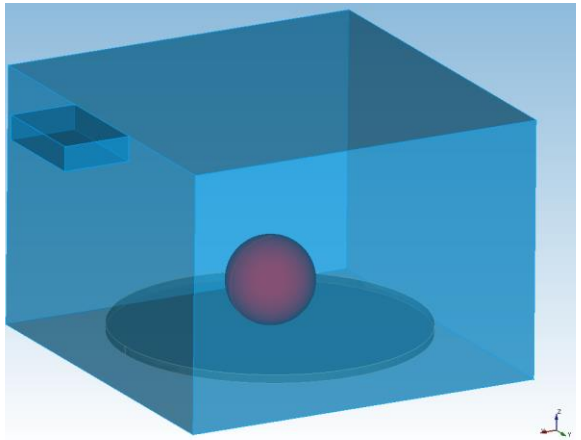


Accurate modelling of coupled electromagnetic-thermal problems

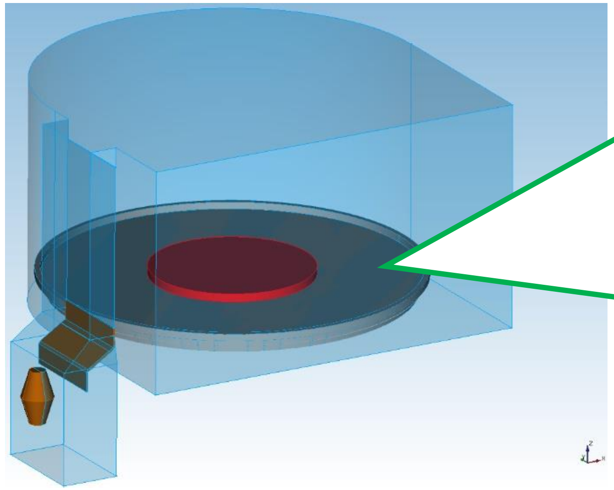
Verification & validation

Simple microwave heating benchmarks & microwave heating phenomena studies*

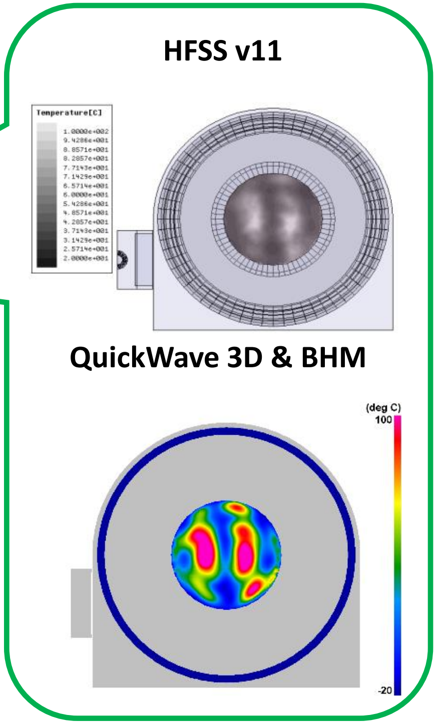
Design & analysis of real-life microwave oven cavities, incl. complicated cavity shapes and advanced feeding system*



- heat transfer & load dynamics
- Load rotation & arbitrary movement during heating
- Source parameters tuning – regime for solid state sources
- Temperature dependence of material parameters

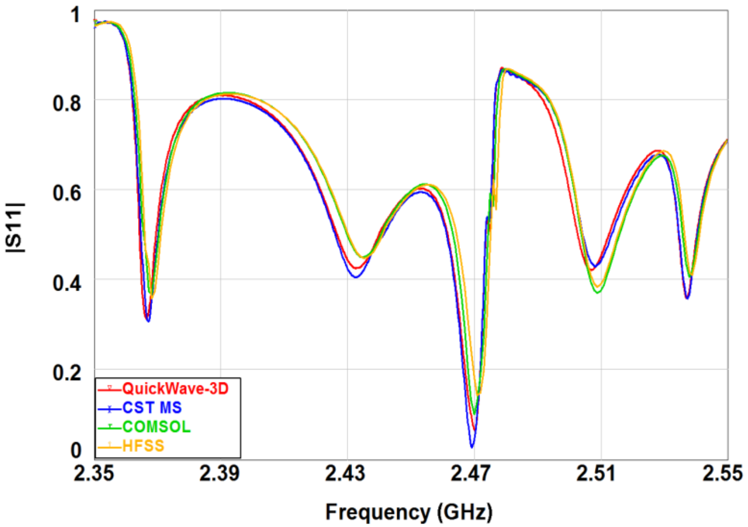


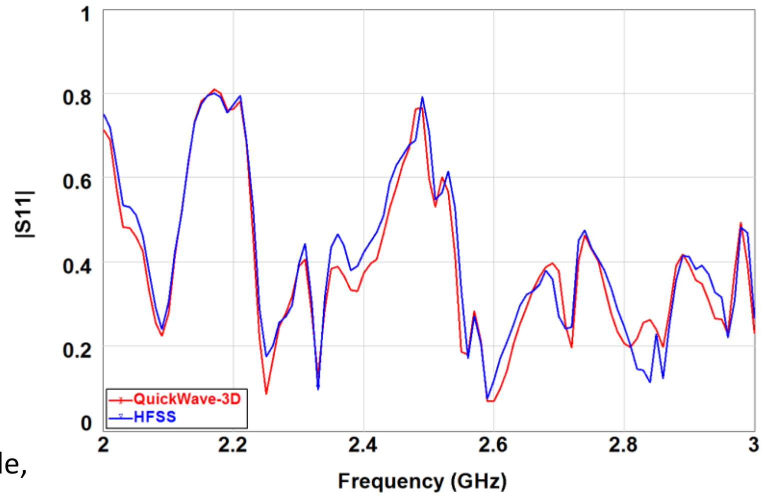
Courtesy of Whirlpool Inc. – Whirlpool MAX oven



Freezing to file the state of the simulation

De-freezing on arbitrary computer & at convenient time





With QuickWave EM computation as fast as 1 min 18s on a low-cost video card – supporting all graphic cards with OpenCL

* Considered by M.Celuch, P.Kopyt & M. Olszewska-Placha in eds. M. Lorence, P. S. Pesheck, U. Erle, *Development of packaging and products for use in microwave ovens*, 2nd Ed. Elsevier in print.

FDTD modelling at the Warsaw University of Technology in 1980-1990s

W.K.Gwarek, "Analysis of an arbitrarily-shaped planar circuit - a time-domain approach", **invited paper**, *IEEE Trans. Microwave Theory Tech.*, vol.33, No.10, Oct.1985.
W.Gwarek, "Computer-aided analysis of arbitrarily-shaped coaxial discontinuities", *IEEE Trans. Microwave Theory Tech.*, vol.36, No.2, Feb.1988.
→ QuickWave 2D launched onto the market by ArguMens GmbH

M.Celuch-Marcysiak & W.Gwarek, "Formal equivalence and efficiency comparison of the FD-TD, TLM and SN methods in application to microwave CAD programs", *Proc. 21st European Microwave Conf.*, Stuttgart, Sept. 1991.
→ FDTD and TLM and SN are formally equivalent but FDTD is computationally more efficient (and opens way to conformal modelling)

PUBLICATIONS IN ENDLESS REVIEWS → DECISION TO PROVE OUR POINT ON THE MARKET
EC SUPPORT via COPERNICUS PROJECT 1994-1996 INTERRUPTED...

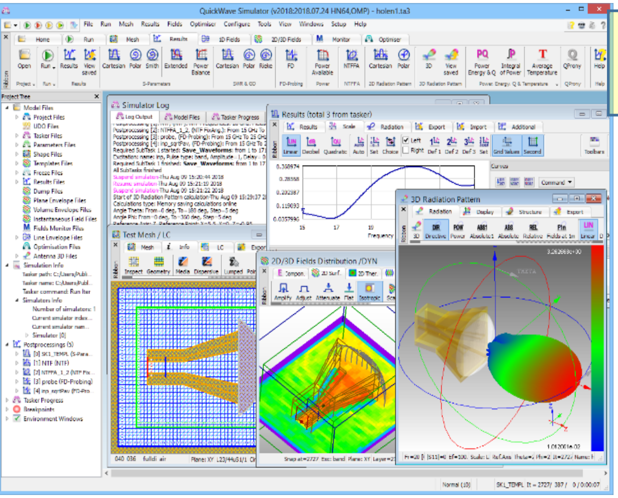
BUSINESS BORN OUT OF OBSTACLES?..

M.Celuch-Marcysiak, "Time-domain approach to microwave circuit modeling: a view of general relations between TLM and FDTD", **invited paper**, *Intl. Journal of Microwave and Millimeter-Wave Computer Aided Engineering*, vol.6, No.1, 1996.
M.Celuch-Marcysiak, W.K.Gwarek, "On the nature of solutions produced by finite difference schemes in time domain", **invited paper**, *Int.Journal of Numerical Modelling*, vol.12, No. 1-2, Jan.-Apr.1999.
M.Celuch-Marcysiak & W.K.Gwarek, "Generalized TLM algorithms with controlled stability margin and their equivalence with finite-difference formulations for **modified** grids", *IEEE Trans. Microwave Theory Tech.*, vol. MTT-43, No.9, Sep.1995.
→ TLM can be made as good as FDTD

International research context:
K.S.Yee, "Numerical solution of initial boundary-value problems involving Maxwell's equations in isotropic media", *IEEE Trans.Ant.Prop.*, vol.14, No.5, 1966.
A.Taflove, M.E.Bodwin, "Numerical solution of steday state electromagnetic scattering problems using the time dependent Maxwell's equations", *IEEE Trans. Microwave Theory Tech.*, vol.33, No.10, Oct.1985.
A.Taflove, S.Hagness, (with chapters co-authored by M.Celuch & W.Gwarek) "Computational Electrodynamics - The Finite-Difference Time-Domain Method", 3rd Edition, Artech House, Boston-London, 2005.

Polish high-tech SME - 24 years on the world's market

Business branches *presented annually at IEEE IMS Show*

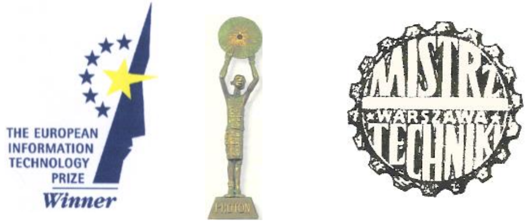


Electromagnetic simulation & design software, 3D & BOR 2D tools

based on 300+ publications by:

prof.W.Gwarek, IEEE Fellow, DML, Pioneer Award

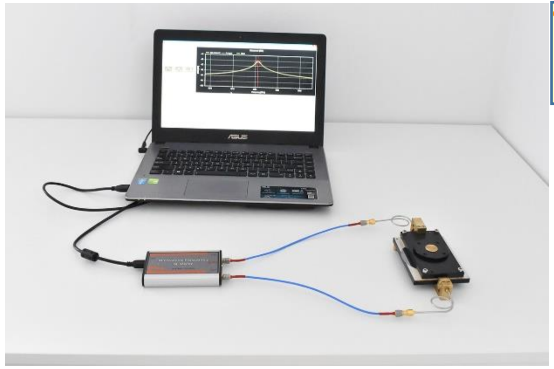
dr.M.Celuch, President of QWED




PREZES RADY MINISTRÓW

przyznaje III nagrodę

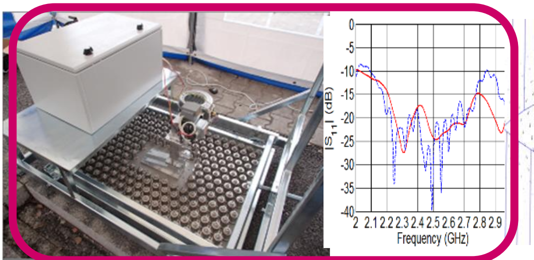
za wybitne krajowe osiągnięcie naukowo-techniczne

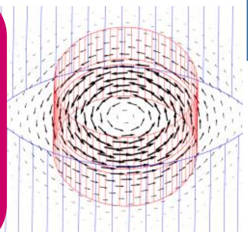


Test-fixtures for precise material measurements

based on 300+ publications

by prof.J.Krupka, IEEE Fellow





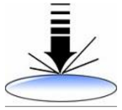
Consultancy & design services based on EM expertise & tools

team of 10+engineers, 4 PhDs, 2 Profs

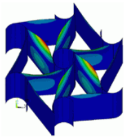
key areas: MW power appliances, customised resonators, antennas &feeds

R&D projects

started with COPERNICUS 1994-1996



FP6 SOCOT – development and validation of an optimal methodology for overlay control in semiconductor industry, for the 32 nm technology node and beyond.



FP6 CHISMACOMB – development, modelling, and applications of chiral materials → EM validation of mixing rules

Eureka E! 2602 MICRODEFROST MODEL – innovative software-based product development tool for simulating and optimising heating and defrosting processes in microwave ovens

SYNTHETIC ENVIRONMENT RESEARCH PROGRAM HIRF

FP7 HIRF SE (High Intensity Radiated Field Synthetic Environment) - numerical modelling framework for aeronautic industry

Eureka FOODWASTE – developing new microwave treatment system for high water content waste

ERA-NET MNT NACOPAN – applications and modelling of nano-conductive polymer composites

PBS Program Badań Stosowanych

NGAM2 – designing an industrial device for thermal bonding of bituminous surfaces with the aid of microwave heating

MMAMA

MMAMA (Microwave Microscopy for Advanced and Efficient Materials Analysis and Production) – accelerating the development of high efficiency solar cells through application and enhancement of material measurement techniques

Nano Bat

NanoBat - developing a novel nanotechnology toolbox for quality testing of Li-ion and beyond Lithium batteries with the potential to redefine battery production in Europe and worldwide.

Current core team

10
people employed

7
consultants cooperating

A happy blend of electromagnetic engineers, multiphysics researchers, IT experts, business analyst, and cross-media specialist

50%
female

Dr. Malgorzata Celuch
President since 2017, VP 1997-2017
- 35 y experience in mathematical, 25 y in management
- Awards for excellence from e.g. Prime Minister of Poland, Rector of WarsawUnivTech

Janusz Rudnicki, MS,
VP for IT
- 22 years of experience in simulation software development

Dr. Marzena Olszewska-Placha,
VP for R&D
- 15 y of experience in simulation-based MHz to THZ design and consultancy
- 4 y experience in research management

Dr. Andrzej Więckowski
Senior in CAD
- 48 years of experience in computer-aided electronic engineering and engineering software development

Prof. Wojciech Gwarek,
President 1997-2017
- 22 years of experience in simulation software development

Dr. Maciej Sypniewski
Senior in CAE
- 48 years of experience in engineering software development and GHz measurements

2021 Finalists

INNOVATION RADAR Prize

TEAMS AWARDS

MISTRZ WARSZAWA TECHNIK

THE EUROPEAN ICT PRIZE WINNER

QuickWave™ skills – becoming a requirement for jobs…

Glassdoor, July 8th,2019

Associate Scientist/Research Engineer

3.7 ★ Associated Universities, Inc. – Charlottesville, VA

Apply on Company Site | Save

2 days ago

Add your resume and apply to jobs with your Glassdoor profile. Create Profile

Job | Company | Rating | Salary

Position Description:

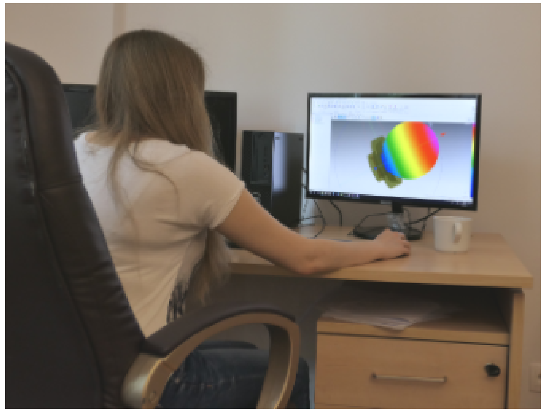
Position Summary

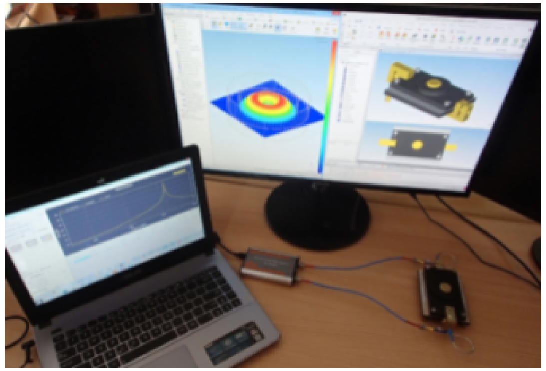
The National Radio Astronomy Observatory's (NRAO) mission is to enable forefront research into the Universe at radio wavelengths. In partnership with the scientific community, we:

- Provide world leading telescopes, scientific software and algorithms and expertise,
- Train the next generation of scientists and engineers, and
- Promote astronomy to foster a more scientifically literate society.

Competency Summary

The successful candidate should have a PhD in Electrical Engineering or Applied physics, and extensive experience in the following fields: low-noise mm/sub-mm wavelength receivers and related technologies; superconducting millimeter-wave electronics; microwave circuit design using modern commercially available software (e.g., CST Microwave Studio, QuickWave, Sonnet EM, Microwave Office, ADS); and cryogenic (4-K) systems. In addition, the candidate should have excellent documentation and communication skills in English, including technical writing and public speaking and the ability to communicate complex ideas effectively to other scientists and engineers with different technical backgrounds.





Careers

QWED is a Polish high-tech SME of 15+ R&D engineers, successfully competing on the international markets with corporations of 10 000+, in the areas of computer electromagnetic simulations and material measurements at GHz frequencies. QWED flagship products are:

- QuickWave electromagnetic simulation software, with supporting modules for thermal phenomena, operated through different Graphical User Interfaces, from the industrial standard Autodesk Inventor Software to FreeCAD-based QW-Modeller
- microwave dielectric resonators including SPDRs defined by the European Standard: IEC 61189-2-721:2015

QuickWave software matches and often outperforms the simulation packages by ANSYS, CST, and COMSOL. QWED resonators are advocated by KEYSIGHT as a valued extension to its Vector Network Analysers but also used in conjunction with VNAs of other test & measurement brands including ANRITSU and Rohde & Schwarz.

Since 2019, QWED operations averaged at 10 resonator units sold per months and one licence transaction per week. The commercial success marked by a recent sale of the 1000th measurement test-fixture is backed up by *premiere classe* scientific research led by 2 state professors and coordinated by 2 PhDs.

We seek a passionate engineer - researcher willing to join in our groundbreaking works and ambitious developments, in the frame of industrial and publicly co-funded R&D projects (including European Horizon Framework) in two focus areas:

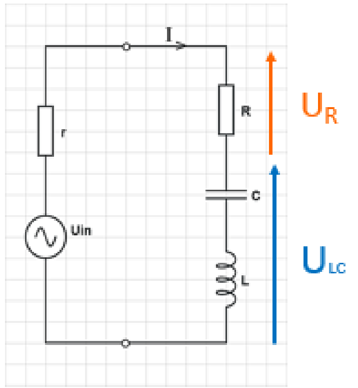
- **multiphysics computer simulations**
- **modelling-assisted measurements of electromagnetic parameters of materials for different industry sectors** (including but not limited to: space, automotive, energy & batteries)

QuickWa
Resonatc
Microwa
Brochure

Electrical & electromagnetic characterisation

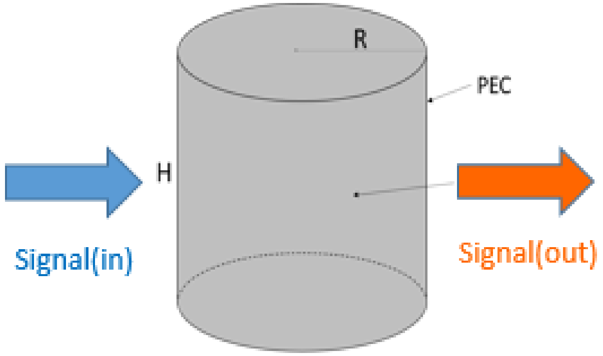
Methodology: design test-fixtures that provide a specific EM response to specific materials

Herein, we focus on resonator methods:

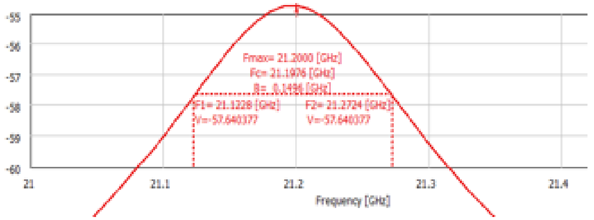


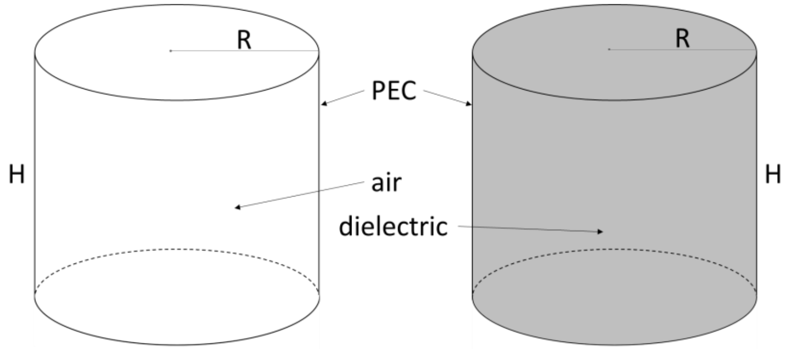
given fixed strength of Uin,
at resonance U_R is strongest (U_{LC}=0)

$$Q = 2\pi \frac{\iiint_V \varepsilon \vec{E}\cdot\vec{E}^* dv}{T\iiint_V \sigma \vec{E}\cdot\vec{E}^* dv} = \frac{\omega\varepsilon}{\sigma} = \frac{1}{Df} \approx \frac{fres}{\Delta f}$$

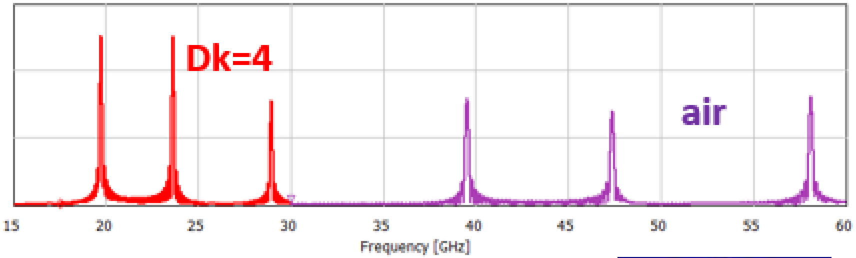


given fixed strength of Signal(in),
at resonance Signal (out) is strongest

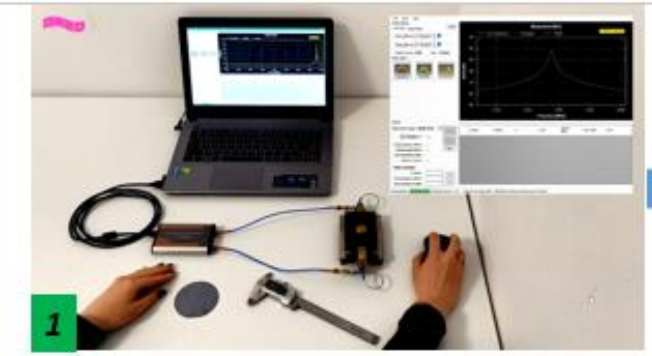


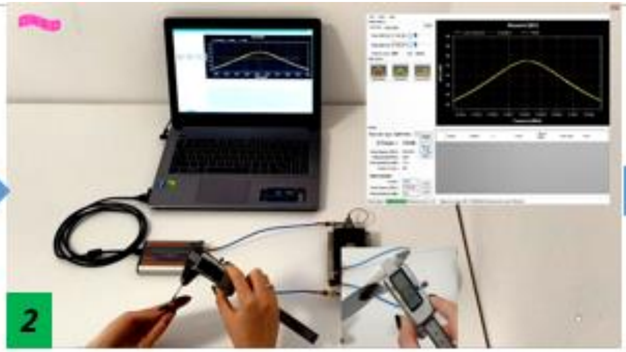


$$f_{r,mnp} = \frac{c}{\sqrt{Dk}}\sqrt{\left(\frac{\kappa_{mn}^{(\prime)}}{\pi R}\right)^2 + \left(\frac{p}{H}\right)^2}$$

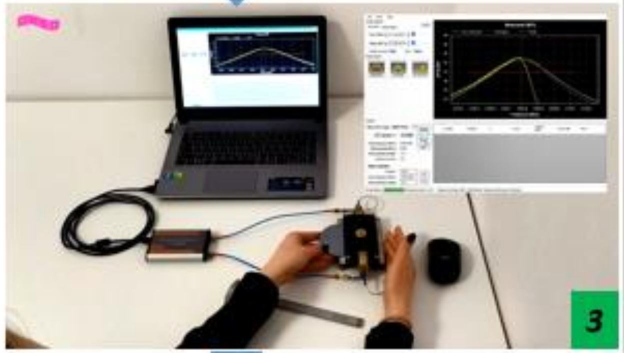


Split-Post Dielectric Resonator (SPDR) – operation





2. Measure thickness of the sample



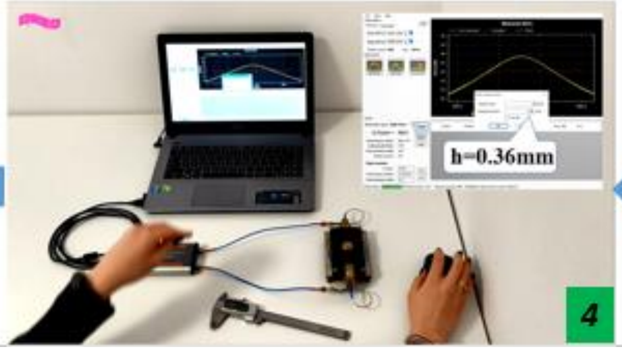
0. Connect the SPDR to Q-Meter using SMA cables.
Connect Q-Meter to PC using USB cable.

1. Measure "empty SPDR" – app invoked measurement.

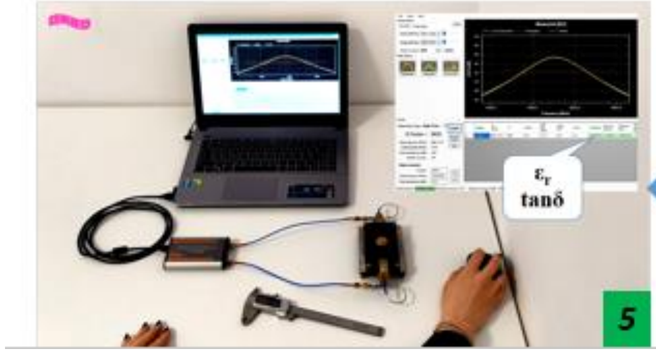
Total measurement time: 30sec

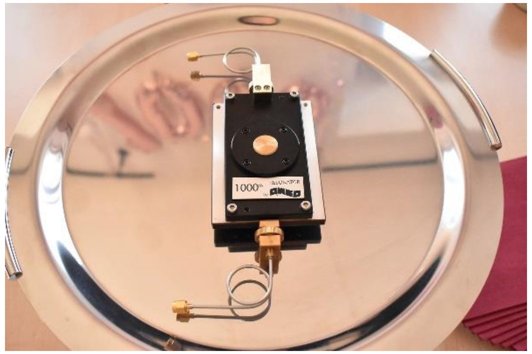
3. Insert the sample into SPDR

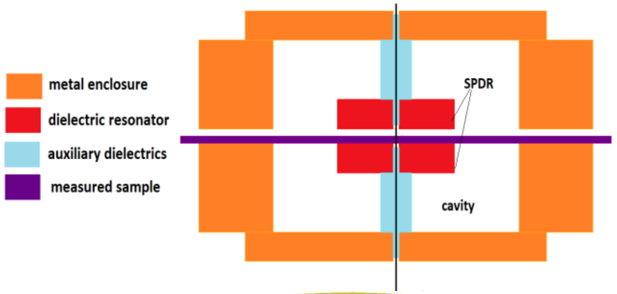
4. Insert the sample thickness into the PC app

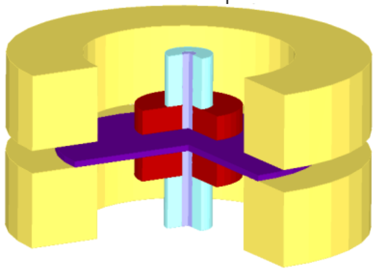


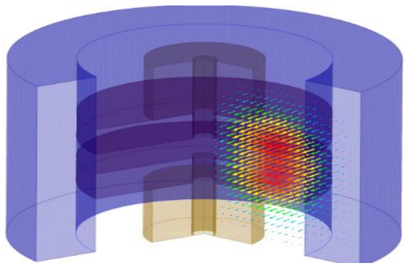
5. Material parameters are extracted automatically



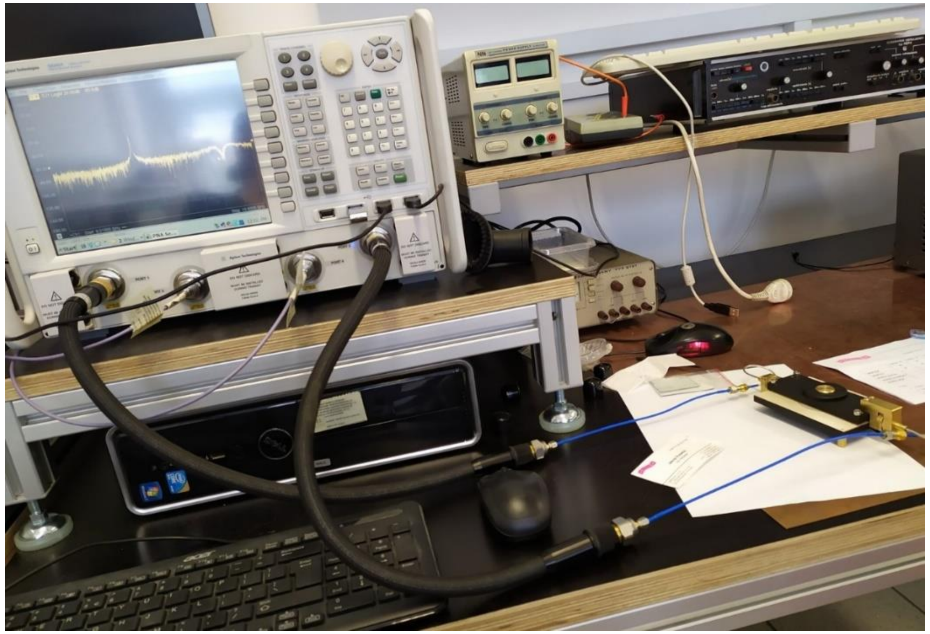






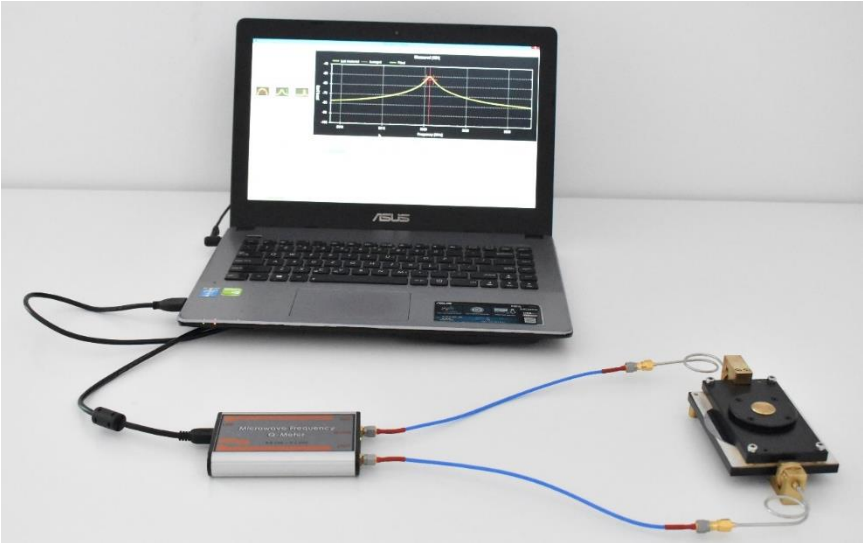


Split-Post Dielectric Resonator (SPDR) – different setups



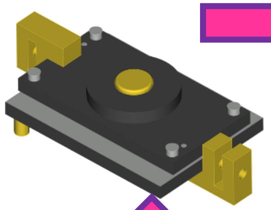
SPDR characterisation performed in labs...

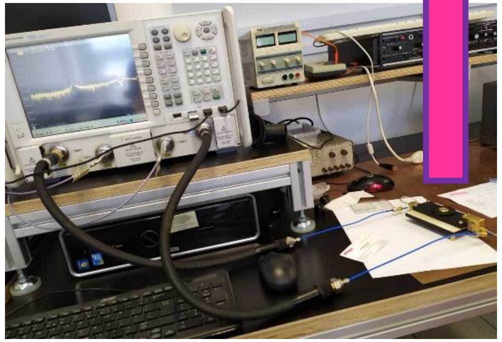
...and at home

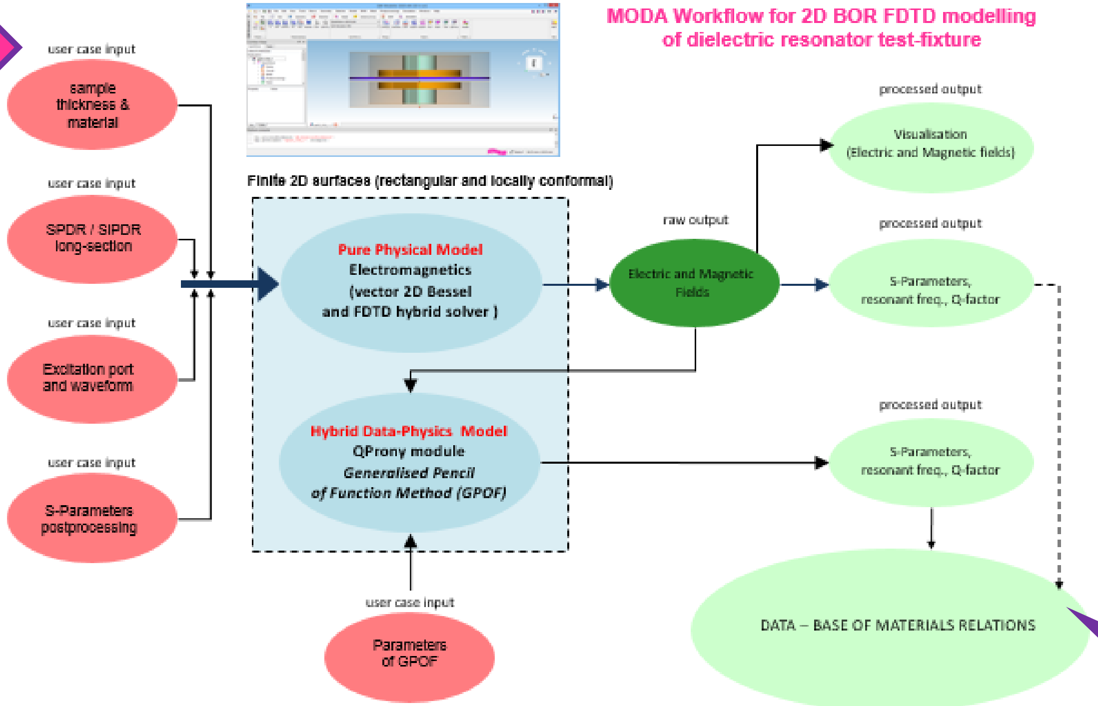


Twinned MODA + CHADA (electrical characterisation in resonator)

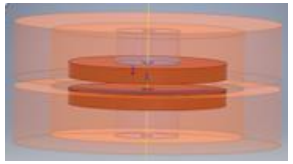
MODA



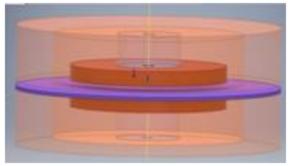


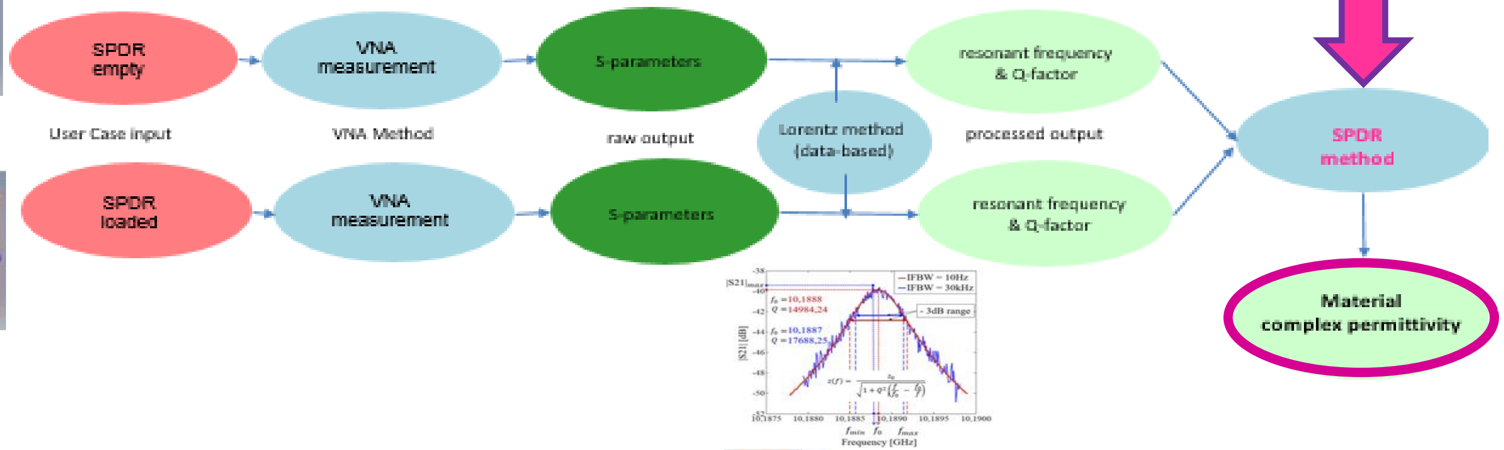


...more physics behind...



CHADA





input from MODA is ESSENTIAL to complete CHADA!

Solution Demonstrator for 5G and energy

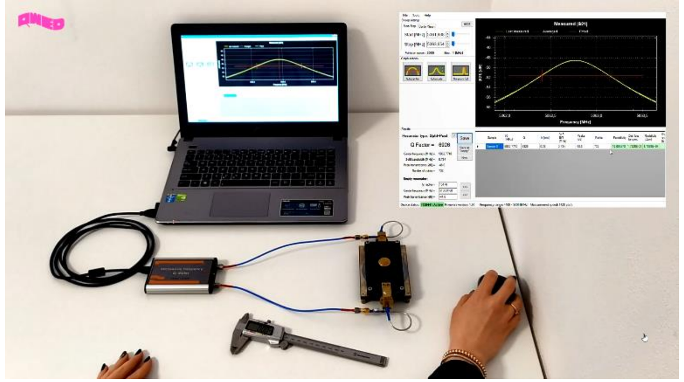
Note: all blocks of this system are being further developed in NanoBat.

The SPDR scanner from MMAMA (for high-resistivity materials) is replaced by a new SiPDR scanner for high-conductivity materials in NanoBat.

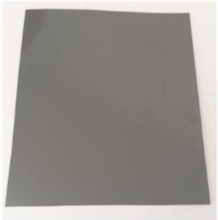
Examples of successful CHADA + MODA use

Application of stand-alone SPDR & SiPDR to graphene anodes & substrates from Pleione (Greece) – characterisation @ 2.45, 5, 10GHz; material used in batteries

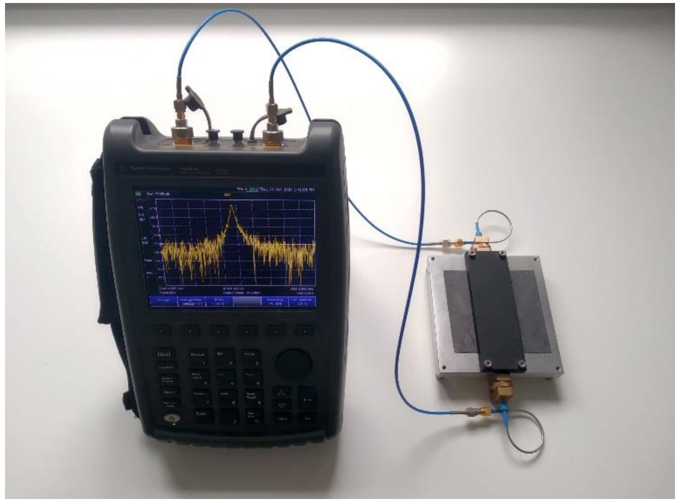
NanoBat project result



Dielectric substrates (*PLEIONE, Greece*)



Sample	2.45 GHz		10 GHz	
	Dielectric constant	Loss tangent	Dielectric constant	Loss tangent
Quartz	4.42	0.000202	4.41	0.000164
Polymer	4.90	0.27403	5.49	0.091955



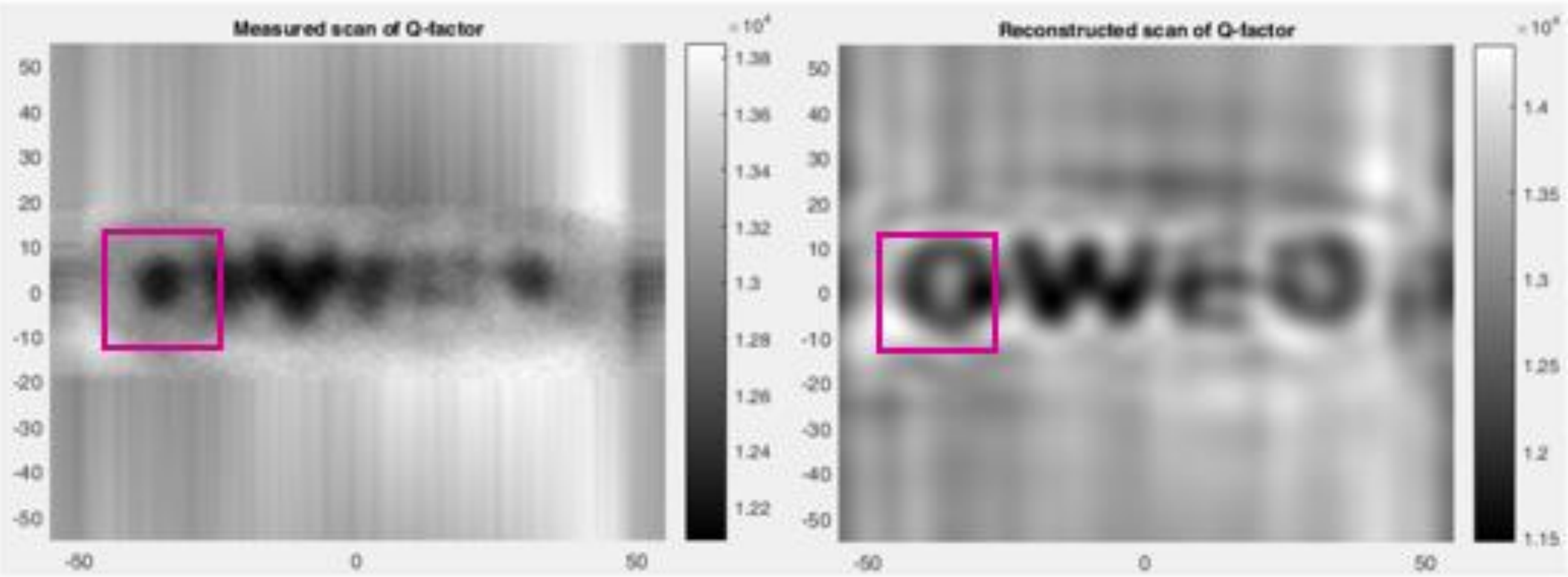
Graphene anodes (*PLEIONE, Greece*)

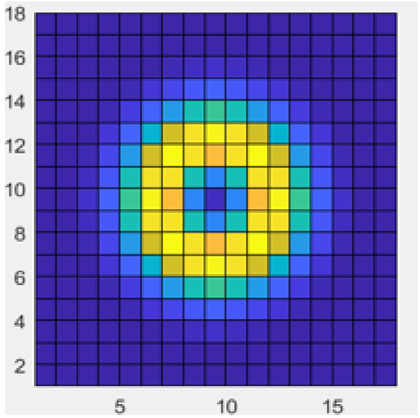
Sample		Surface resistance [Ω/□]
GNP on quartz	Edge	21.485
	Centre	21.020
GNP on polymer	Edge	90.167
	Centre	25.557

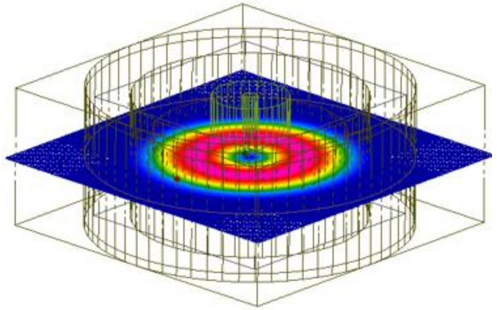
Examples of successful CHADA + MODA use

MMAMA project result

Application of SPDR scanner to patterned PEDOT:PSS (MateriaNova, Belgium) – imaging @ 10GHz, material used in photovoltaics



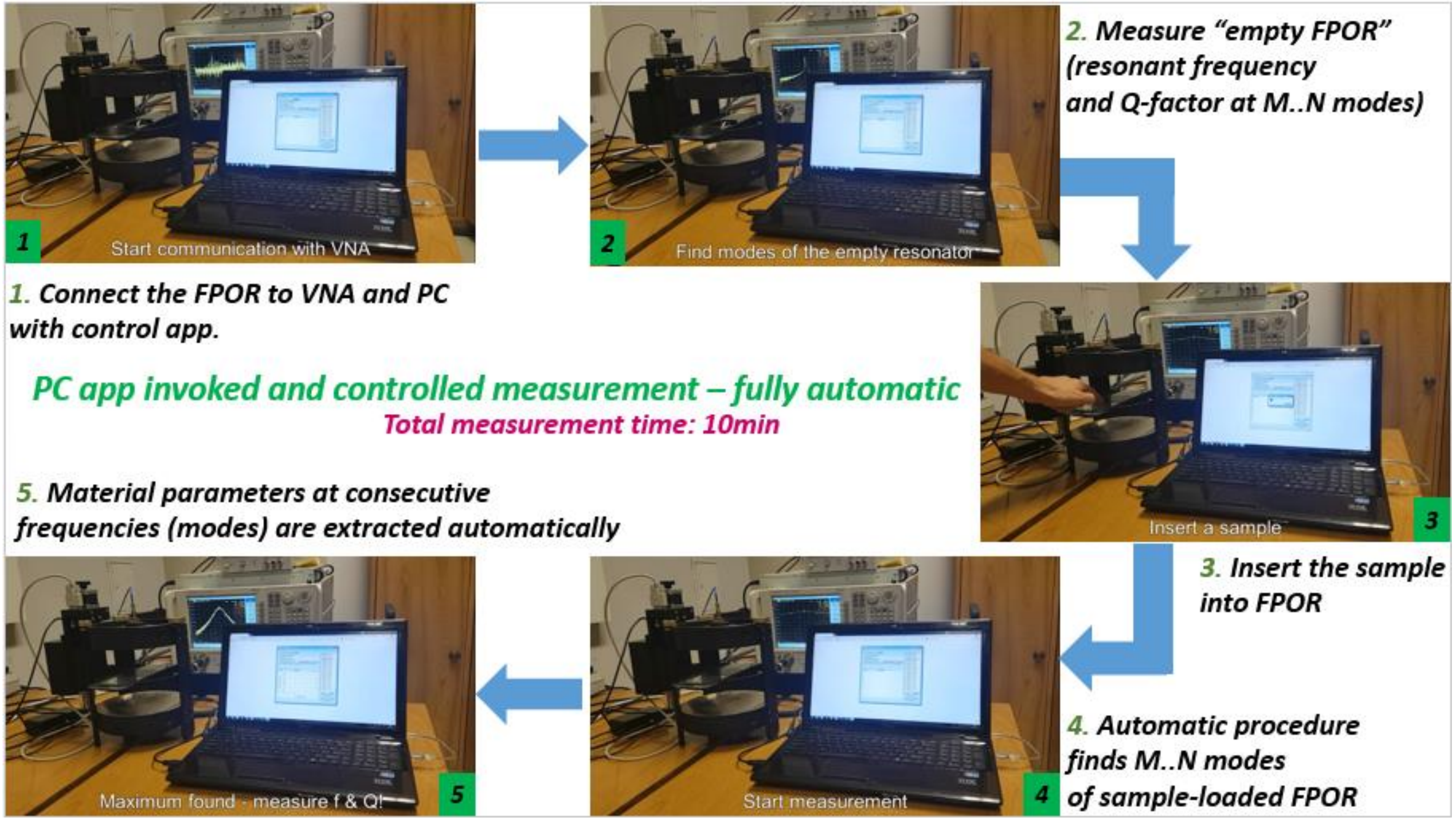


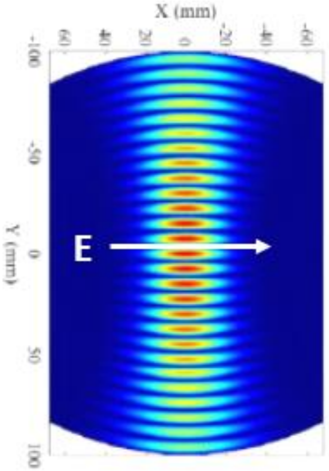


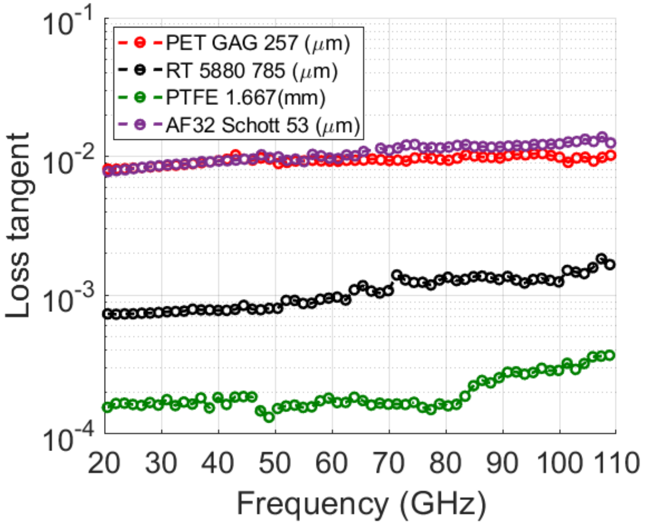
sample resistivity (measured Q-Factor) scan with QWED 10GHz SPDR scanner in H2020MMAMA project

image further post-processed using SPDR field pattern simulated in QuickWave

Application to other test-fixtures: Fabry-Perot Open Resonator

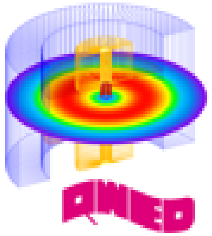






QWED research & market interests

commercial since 1997
QuickWave Simulation Software
~1000 licences implemented

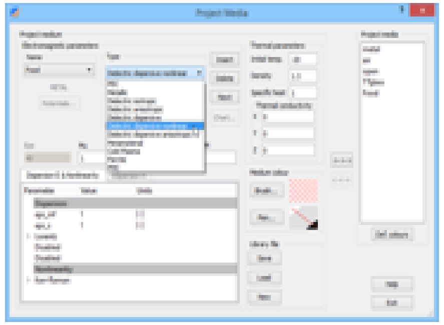


applicator design
& model
for parameter extraction

Modelling
(EM, MW, multiphysics,...)
- waves in free space is "easy" Maxwellian
- wave interaction with matter is "complicated"...

Material measurements

accurate material parameters (constitutive relations)



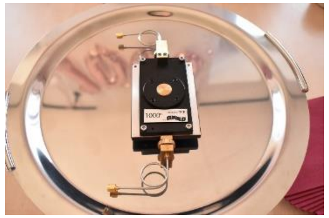
Open Platform Examples & Tools

QW-Modeller for QuickWave
Free general purpose 3D CAD modeller for QuickWave

Open Platform Examples:

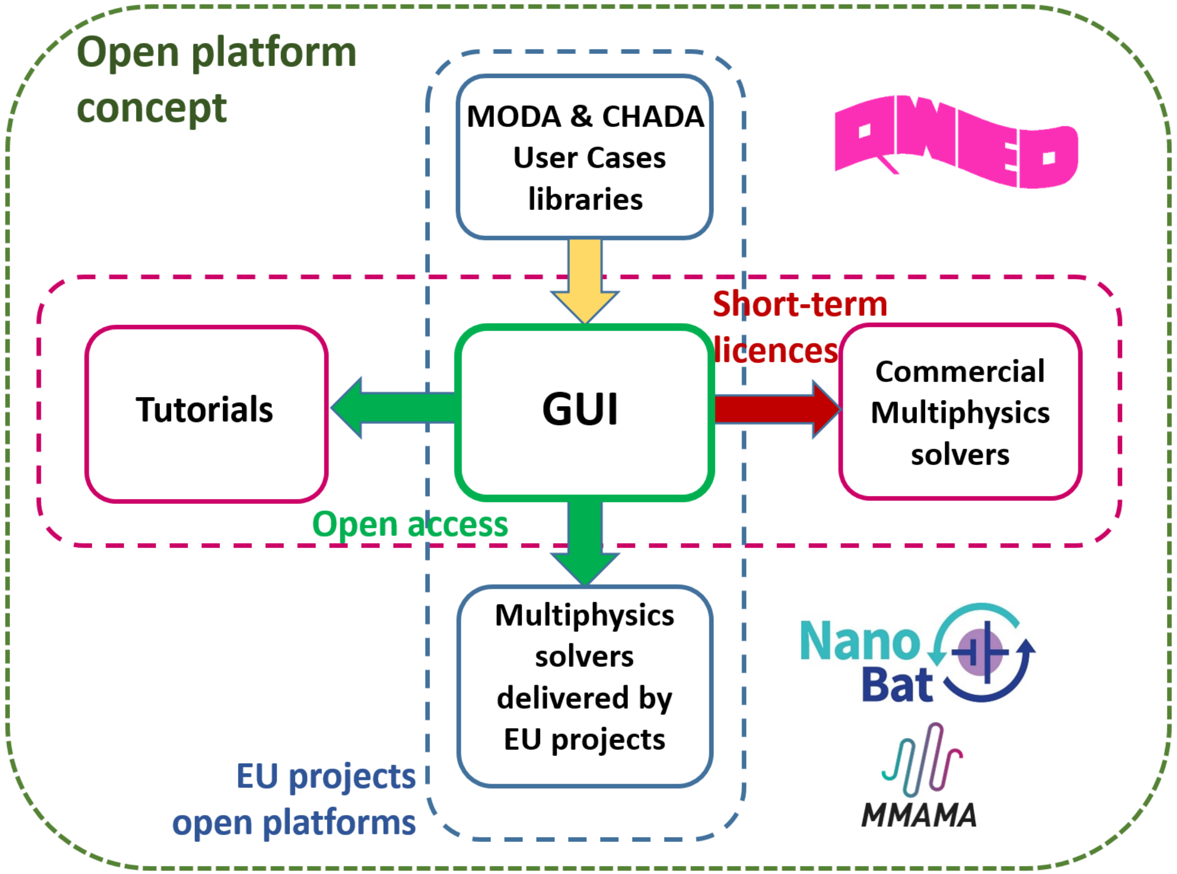
SMM tip presented at Numerical Electromagneti

commercial resonator test-fixtures since 2001
1000th unit sold in 2020



European Standard:
IEC 61189-2-721:2015

Open Platform with MODA & CHADA libraries



- ✓ **Interoperable, licence-free, time-unrestricted CAD-based GUI**
- ✓ **Tutorials** – teaching and project's results dissemination
- ✓ **Library of modelling examples** – documented in MODA format, incl. related CHADAs
- ✓ **Physics-based solvers** - solvers coming from EU projects or other initiatives, willing to provide their tools as open-access.
- ✓ **Data repositories** – linked through reading and processing the data in text files exported by GUI.

EMMC Task Group proposal

Version 2, February 2021

by Marzena Olszewska-Placha and Malgorzata Celuch (QWED)

Focus Area: ***Model Development (also Software)***

Linking and Coupling Computational Chemistry to Electromagnetics

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NanoBat No 861962.

(website: www.nanobat.eu)

Simulations conducted with QuickWave EM software, developed & commercialised by QWED.

THE EUROPEAN INFORMATION TECHNOLOGY PRIZE Winner

The designs of QWED resonators for material measurements are based on:

J. Krupka, A. P. Gregory, O. C. Rochard, R. N. Clarke, B. Riddle, and J. Baker-Jarvis, "Uncertainty of complex permittivity measurements by split-post dielectric resonator technique", *J. Eur. Ceramic Soc.*, vol. 21, pp. 2673-2676, 2001.

J. Krupka and J. Mazierska, "Contactless measurements of resistivity of semiconductor wafers employing single-post and split-post dielectric-resonator techniques," *IEEE Trans. Instr. Meas.*, vol. 56, no. 5, pp. 1839-1844, Oct. 2007.

T. Karpisz, B. Salski, P. Kopyt, and J. Krupka, "Measurement of dielectrics from 20 to 50 GHz with a Fabry–Pérot Open Resonator," *IEEE Trans. Microw. Theory Tech.*, vol. 67, no. 5, pp. 1901–1908, May 2019, doi: 10.1109/TMTT.2019.2905549.

Scenarios of microwave medical applicators from Per O. Risman, Microtrans AB & Malardalen University, Sweden.

Actions & values of coupling Computational Chemistry to Computational EM

Joint projects (incl. student apprentice & summer jobs)

1. Material libraries (added data bases)

2. Computational chemistry solvers launched from the Platform (added tools)

3. Materials parameters calculated off-line (added services)

Strategic:

"Materials by Design" for Electronic Design for GHz to THz applications

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