ELECTRONIC MATERIALS AND APPLICATIONS (EMA 2020)
ORGANIZED BY THE ACERS ELECTRONICS AND BASIC SCIENCE DIVISIONS
January 22 – 24, 2020 | DoubleTree by Hilton Orlando at Sea World Conference Hotel | Orlando, FL, USA

# Exploring synergies between electronic material measurements and modeling

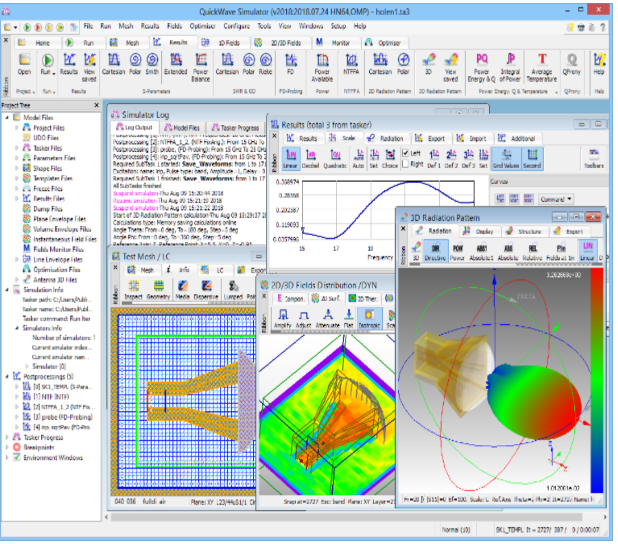
**Malgorzata Celuch*, Marzena Olszewska–Placha, Janusz Rudnicki**

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

**S12 – Electronic Materials Applications in 5G Telecommunications**

# Polish high-tech SME - 23 years on the world’s market

## Business branches *presented annually at IEEE IMS Show*




### QuickWave Electromagnetic Design & simulation software,

**3D & BOR 2D & multiphysics modules**

**based on 300+ publications by:**

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

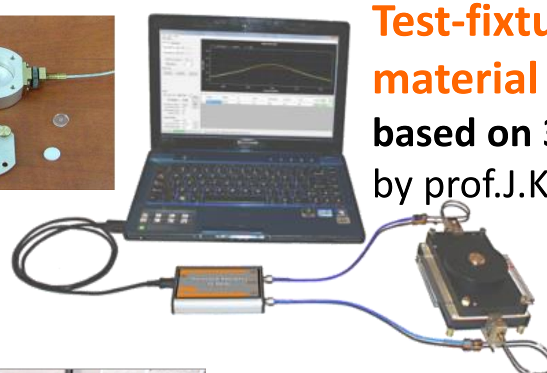
dr.M.Celuch, President of QWED



### Test-fixtures for precise material measurements

**based on 300+ publications**

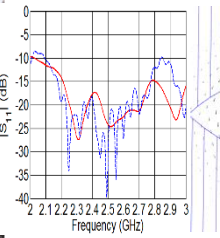
by prof.J.Krupka, IEEE Fellow

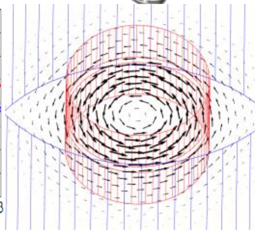



### Consultancy & design services based on EM expertise & tools

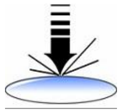
team of 10+engineers, 4 PhDs, 2 Profs

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

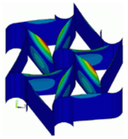


## R&D projects



**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

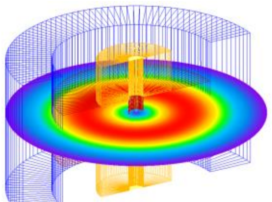
**NGAM2** – designing an industrial device for thermal bonding of bituminous surfaces with the aid of microwave heating

MMAMA

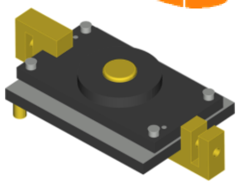
**MMAMA** (Microwave Microscopy for Advanced and Efficient Materials Analysis and Production) – accelerating the development of high efficiency solar cells through application and enhancement of material measurement techniques

# My message for today (*sorry if sounds trivial!*)

Modelling & measurements are not two separate worlds.
Exploring synergies is where QWED sees the future.



**applicator design**
**& model**
**for parameter extraction**

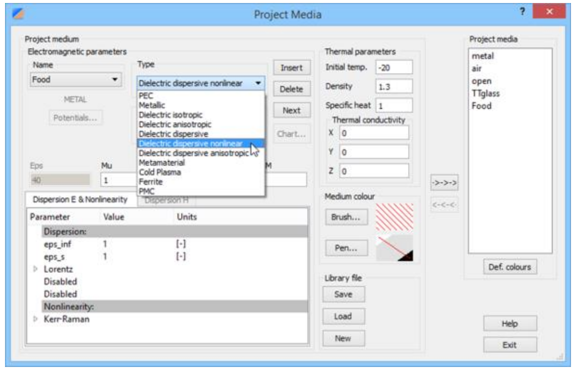


## Modelling
## (EM, MW, multiphysics,...)

- **waves in free space is "easy" Maxwellian**
- **wave interaction with matter is "complicated"...**

## Material measurements

**accurate material parameters (constitutive relations)**

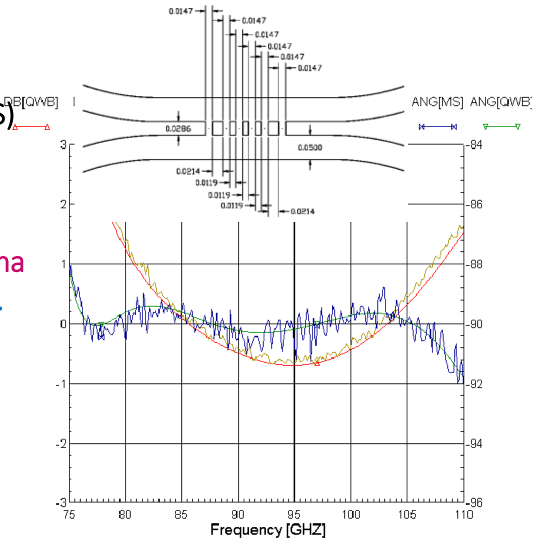


# Electromagnetic modelling and design – antennas & feed systems

## QuickWave-3D: world's recognised 3D EM simulation tool

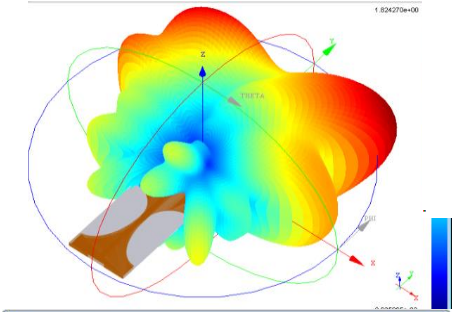
Space research:
NASA related laboratories:
National Radio Astronomy Observatory (VA US),
Jet Propulsion Laboratory (CA US)
Universities:
CALTECH (US), Chalmers (S), etc.

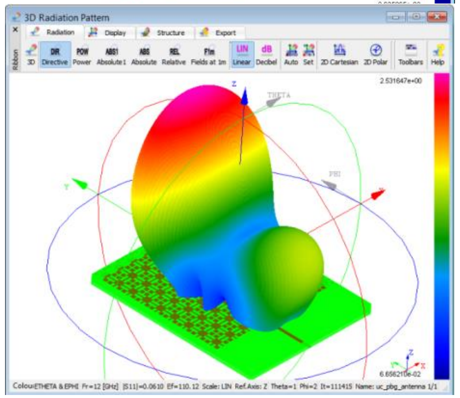
Antenna feed systems designed by NRAO



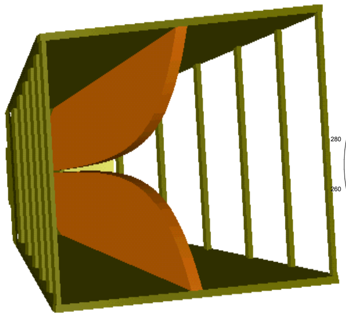

QuickWave 3D results at NRAO, see: ALMA Memos 381, 343, 325, 278.

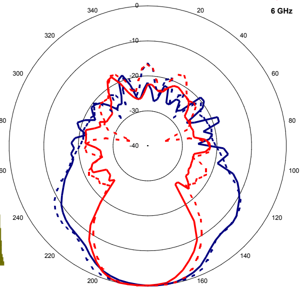
Balanced antipodal Vivaldi antenna & 3D radiation pattern at 10 GHz.





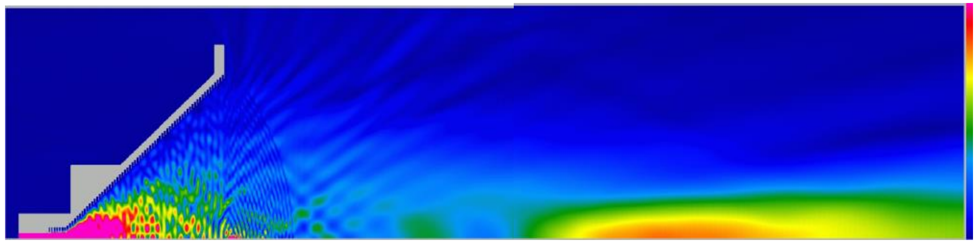

Aperture-coupled patch antenna on uniplanar photonic bandgap substrate & its radiation pattern at 12 GHz.



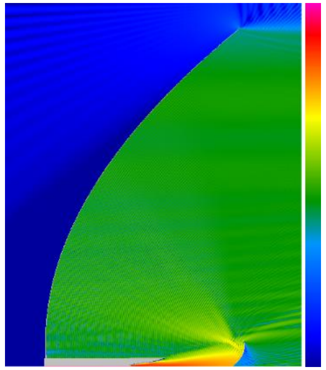


Pyramidal horn antenna for military surveillance measured (courtesy prof.B.Stec) & simulated patterns

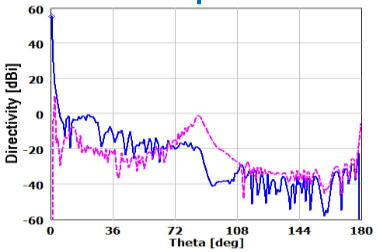
## QuickWave BOR: unique on the market & ultrafast tool for axisymmetrical structures

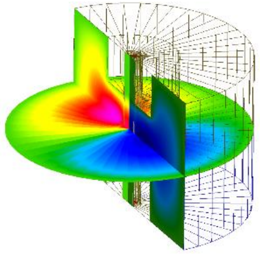


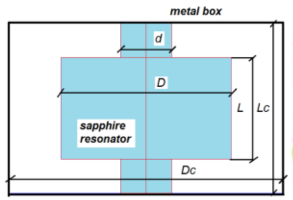
Antennas as large as 2600 λ in diametre on cheap PC

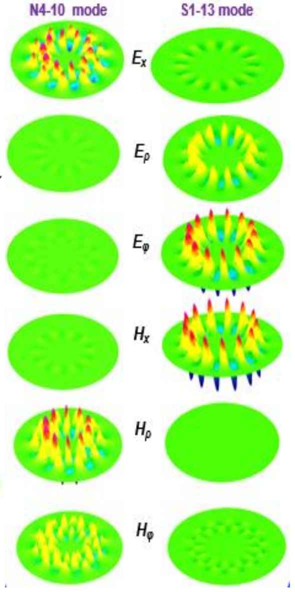


Insight into EM near-field helps explain causes of undesired performance

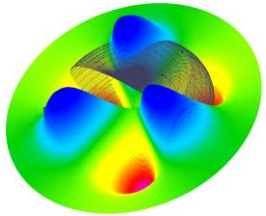


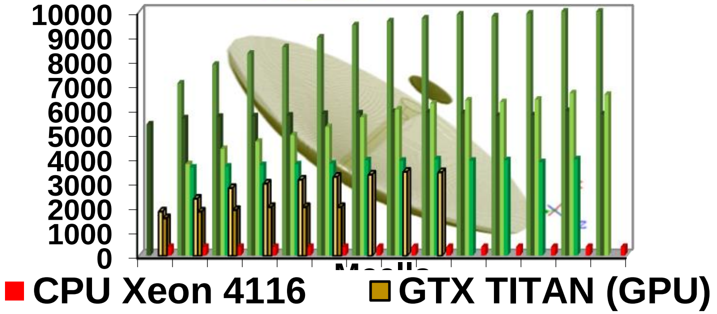



BOR resonators (incl. whispering gallery modes)



QuickWave is optimised for speed plotted in (Mcells/sec), runs on professional & low-cost video cards:




**Pioneering background:**
W.Gwarek, *IEEE Trans. MTT*: vol.33 Oct.1985; vol.36 Feb.& Apr. 1988.

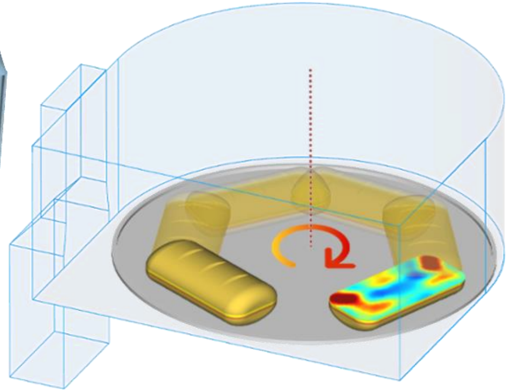
**Key developments:**
M.Celuch & W.Gwarek, *IEEE Trans. MTT*, vol.43 Sep.1995, vol.41 May1993, vol.45 May1997, vol.51 Aug.2003; *EuMC* 1991-1997; *IEEE IMS* 2001-2004.

**Reviews:** *IEEE Microwave Mag.*, Dec.2008 & Apr.2010; *IJMPEE* vol.41 2007.

# Electromagnetic modelling & design – high MW power applications

## Modelling of MW heating effects in domestic oven

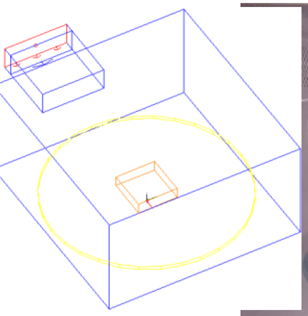
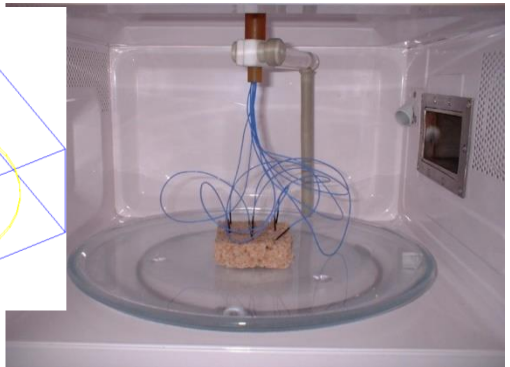
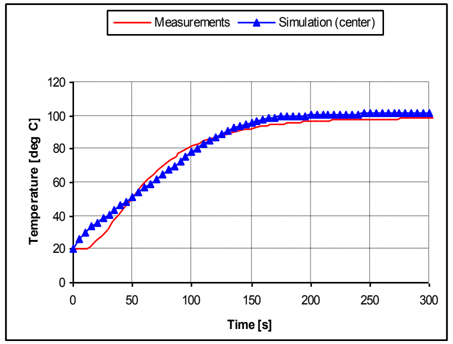
Full-wave EM simulation & heat transfer & load dynamics
Load rotation & arbitrary movement during heating
Source frequency tuning – regime for solid state sources
Temperature dependence of material parameters

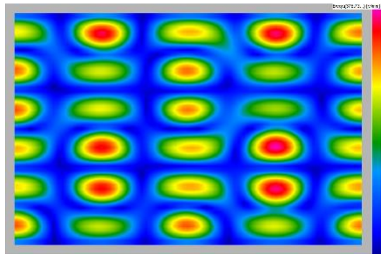
Whirlpool Max oven

Considered by M.Celuch & P.Kopyt in eds. W. Lorence and P. S. Pesheck, *Development of packaging and products for use in microwave ovens*, 1st edition Woodhouse CRC Press 2009, 2nd Ed. Elsevier in print.

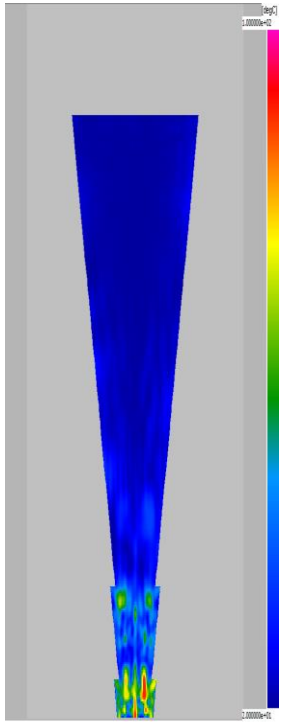
QuickWave modelling of heating confirmed by real-life experiments – joint work of QWED and WUT in Eureka E!2602 project

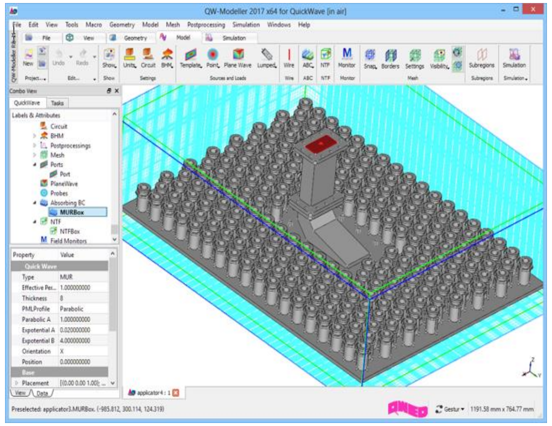

## Free-fall waste processing on ships (Eureka FOODWASTE)



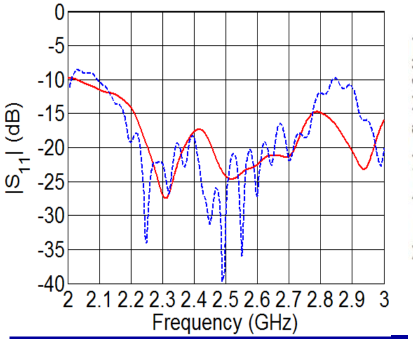
E-field in horizontal & vertical cut

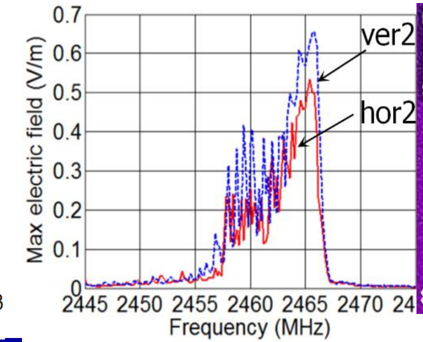


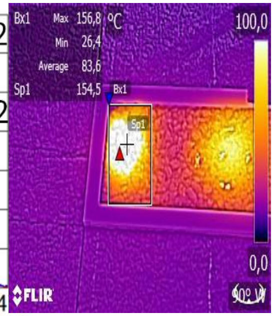
## High power applicator for MW treatment of bituminous surfaces (road repair, NGAM project)

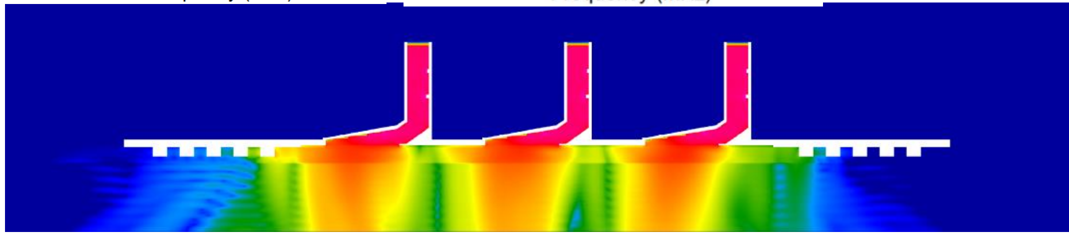



convenient CAD input









System of three MW power applicators with feeding system and leakage preventing chokes: designed, manufactured, tested

B.Salski et al., *IEEE MTT Trans.*, vol.65, Sep.2017.

# Acknowledgements

The work presented has received funding from the

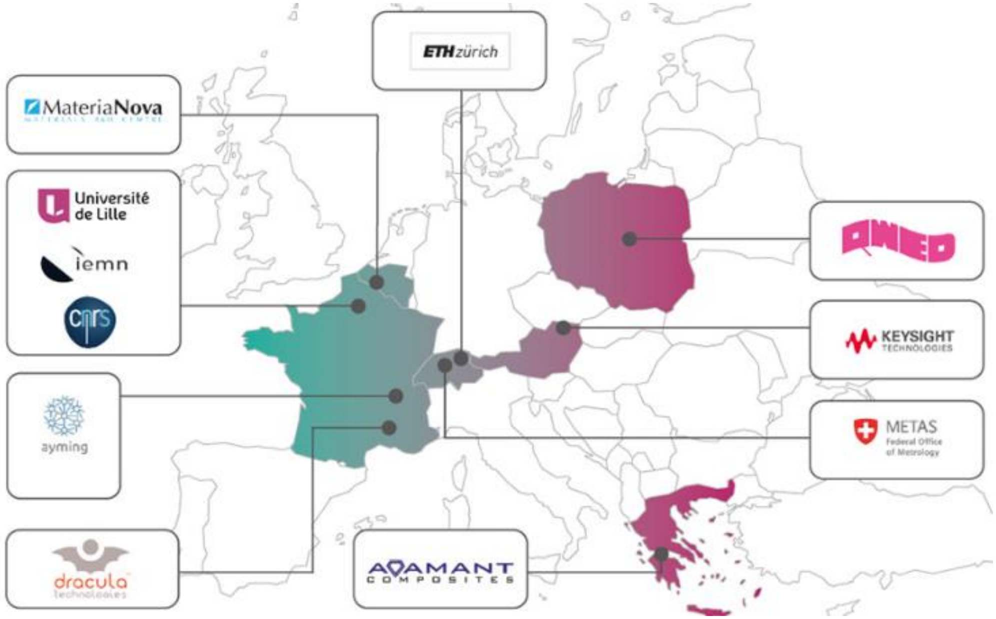
*European Union's Horizon 2020*

research and innovation programme (H2020-NMBP-07-2017)

under grant agreement

*MMAMA n°761036*.

(website: www.mmama.eu)




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

**The original designs of QWED resonators for material measurements were from Prof. Jerzy Krupka, e.g.:**

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.

**Microwave heating scenarios & concepts by Per O. Risman, Microtrans AB & Malardalen University, Sweden.**

# Outline

- Electromagnetic modelling as a basis for precise material measurements
- Split-post dielectric resonator (SPDR): why it has become a standard
- Other types of dielectric resonators
- SPDR measurements of larger surfaces & resolution enhancement
- "Transfer of technology" from other application & the applications themselves:
    - "*near field imaging*" from MW heating
    - multiphysics modelling of MW heating
    - common CAD interfaces
    - sub-cellular models in FDTD (*hints*)
    - "*near field imaging*" in antenna design
- Modelling of SMM tips for material measurements at nano-scale
    - unconventional (but constructive) definitions of impedance and S-matrix
- Conclusions

# Dielectric resonator methods for material measurements

SUT of $\varepsilon_s = \varepsilon_s' - j\,\varepsilon_s''$ is inserted into DR:
resonant frequency changes from $f_e$ to $f_s$
Q-factor changes from $Q_e$ to $Q_s$.

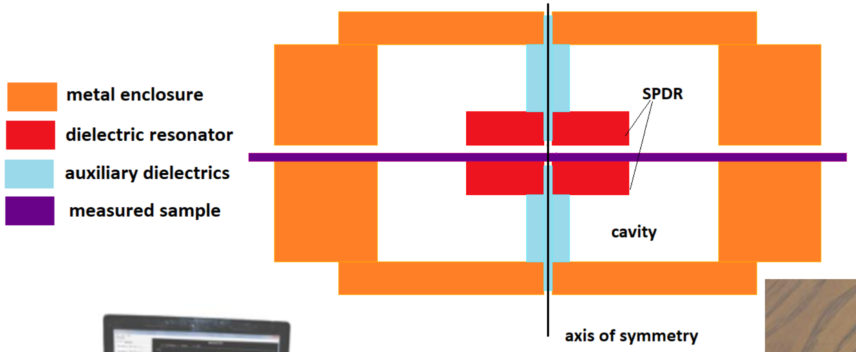
$$\frac{f_e - f_s}{f_e} \approx \frac{h}{2C} \iint_S \left[ \varepsilon_s'(x,y) - 1 \right] \left| E(x,y) \right|^2 dS$$

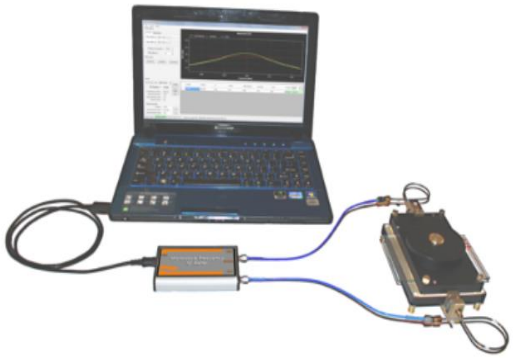
$$\frac{1}{Q_s} - \frac{1}{Q_e} \approx \frac{h}{C} \iint_S \varepsilon_s''(x,y) E^2(x,y)\, dS$$

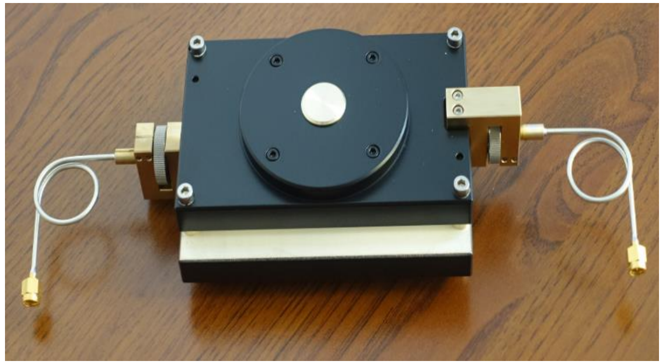
$$C = \iiint_V \left| E(x,y) \right|^2 dV$$

field assumed invariant in *z*-direction
*S* is called the DR's *head*
**sign ≈** reflects field patern changes caused by SUT

**Most popular example: Split-Post Dielectric Resonator**



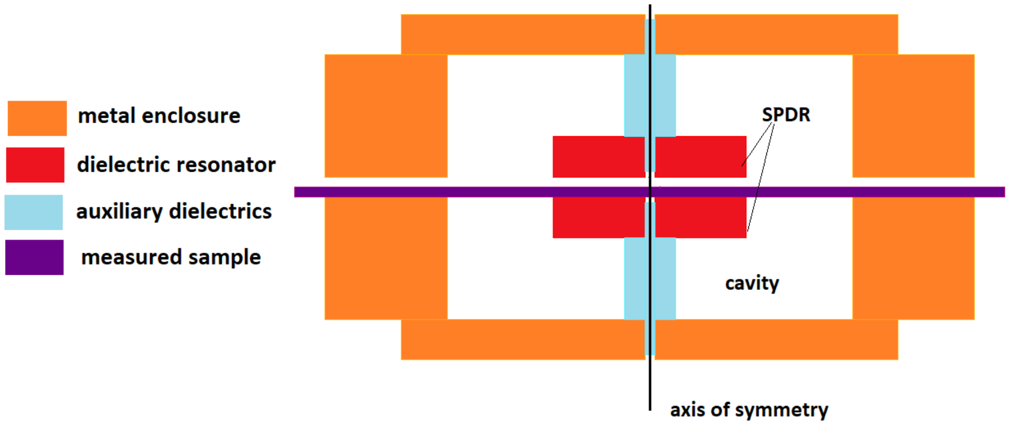



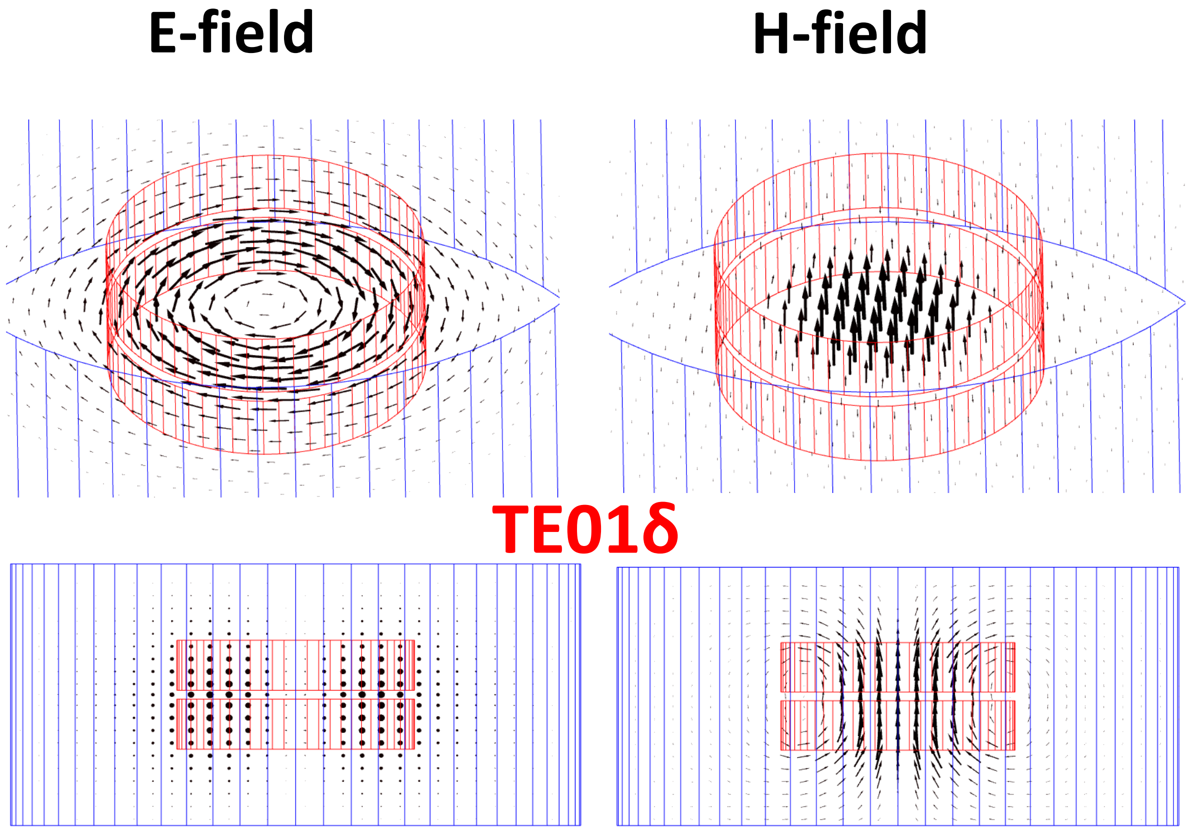


calibration
(only once, upon manufacturing!)
minimises efects of:

field variation in *z*
field changes due to SUT
manufactruing tolerances

# Fields in SPDR

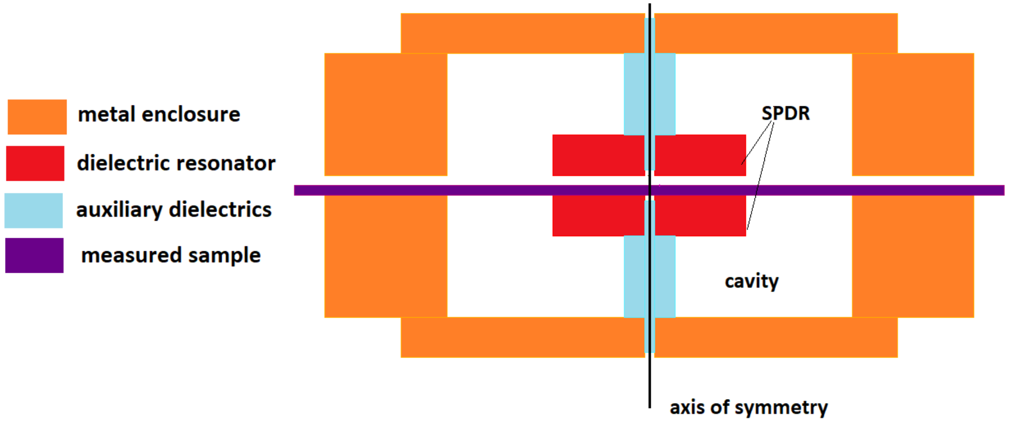


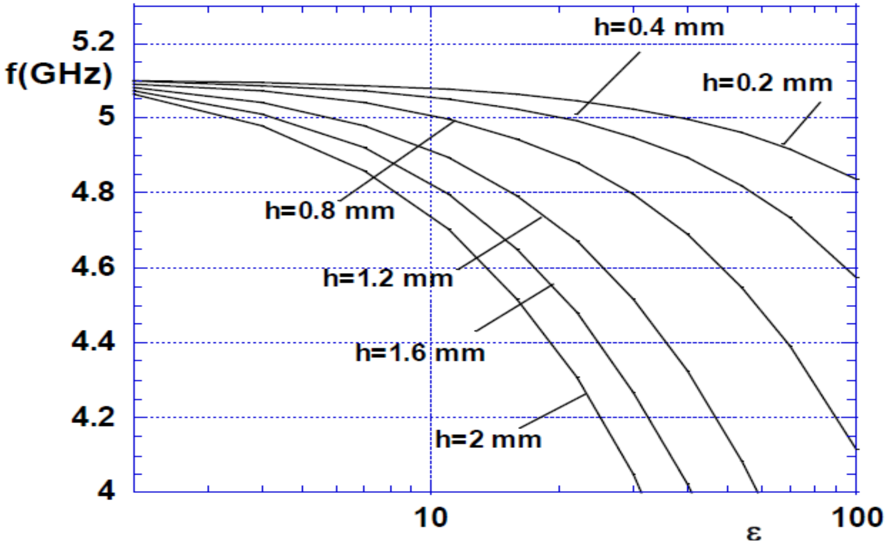




- resonant mode with EM fields mostly confined in and between those ceramic posts → minimial losses in metal enclosure
- H-field is only vertical at the side wall of the enclosure → only circumferential currents in side wall → no radiation through slot
- E-field tangential to SUT → air slots between SUT and posts have negligible effect
- **easy SUT insertion through slot, no dismatling, NDT method**
- all EM energy injected through the coupling loops in contained within in the SPDR “head” (inside the enclosure)
- an estimated 95% of energy confined in and between the ceramic posts
- **calibration only once, at manufacturing**

# Accuracy of SPDR measurements

QWED SPDRs for: 1.1, 1.9, 2.5, 5, 10, 15 GHz




accuracy for $\varepsilon$ typically 0.3%

measurable losses tanδ ~6 $10^{-5}$

$$\Delta\varepsilon/\varepsilon=\pm(0.0015 + \Delta h/h)$$

$\Delta\tan\delta=\pm2*10^{-5}$ or $\pm0.03*\tan\delta$ whichever is higher

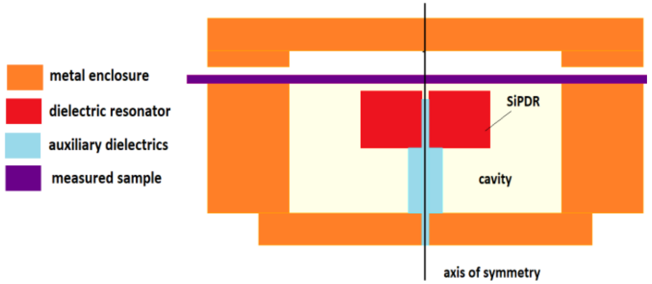
## → European Standard: IEC 61189-2-721:2015

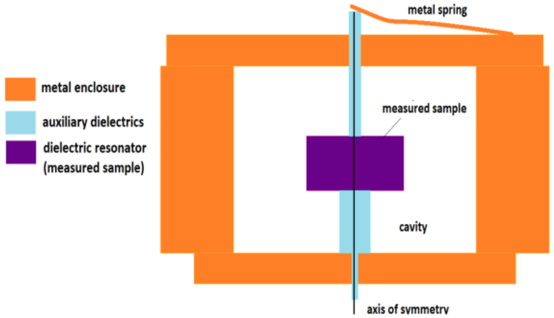
**Limitations** ***(which we are currently addressing...)*:**

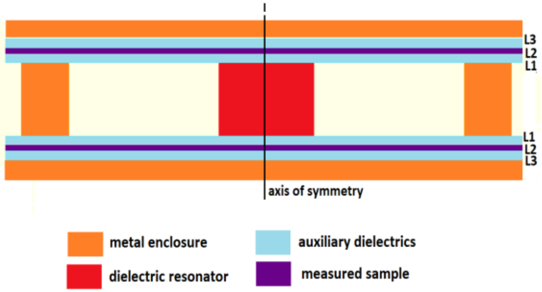
- **SUT thickness - slot size 0.6..6 mm**
- **SUT lateral min size ("absolute" EM constraint) - 14..120 mm**
- **spatial resolution 14..120 mm**
- **SUT lateral max size (mechanical construction) – 40..150 mm**

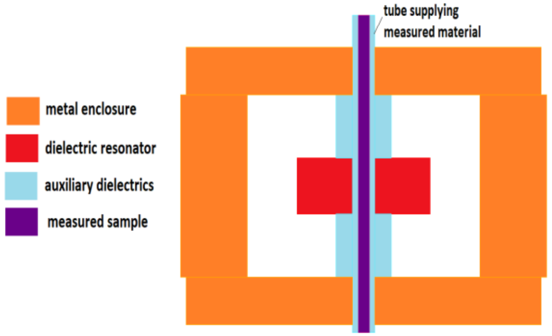
| | Conductivity [1/(Ωm)] | Resistivity [Ω cm] | Surface resistivity [Ω/sq] |
|---|---|---|---|
| Range od SPDR applications | from $10^{-2}$ to 1 | from $10^2$ to $10^4$ | from 5 $10^3$ to $10^6$ |
| Range of SiPDR applications | from 1 to $10^7$ | from $10^{-5}$ to $10^2$ | from 2 $10^{-4}$ to 5 $10^3$ |
| Sapphire | > 5 $10^6$ | | |

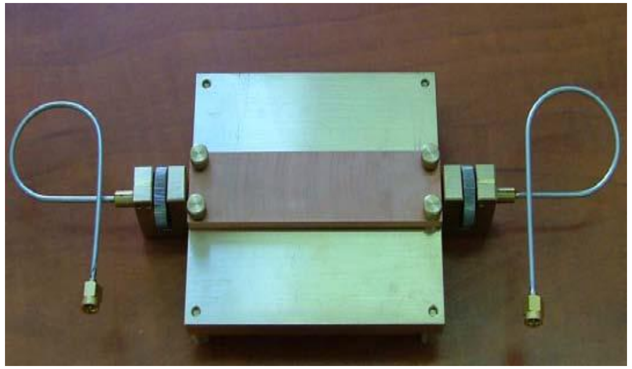
# Other types of dielectric resonators (TE01δ)

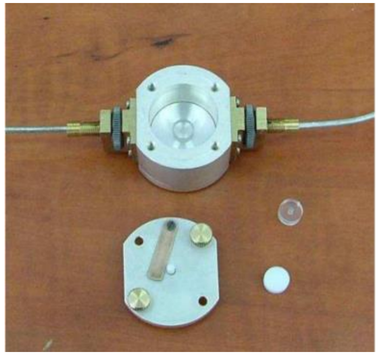


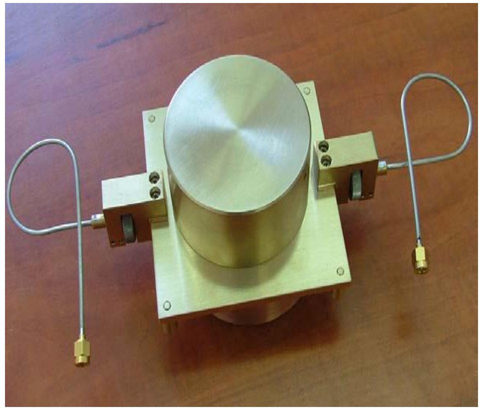



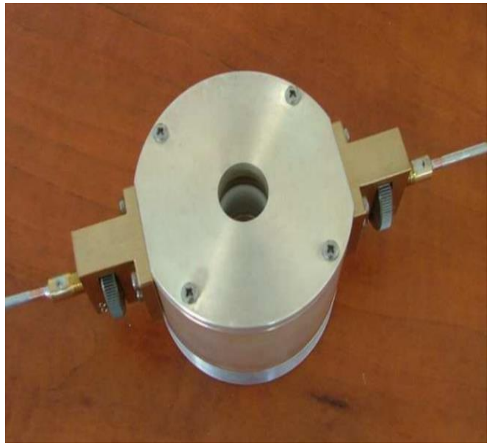









**single-post**
**resistive sheets**

**cavity**
**resonating SUT**
**ultra-low-loss SUTs**

**sapphire**
**metal SUTs**

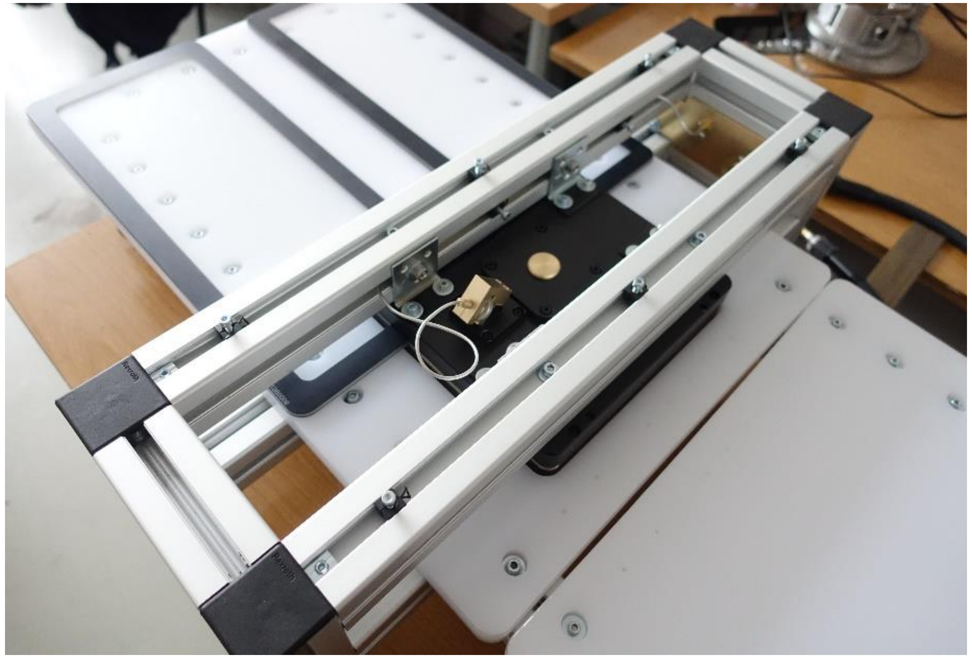
**liquids & powders**
***can also heat***

# Surface scanning with SPDR

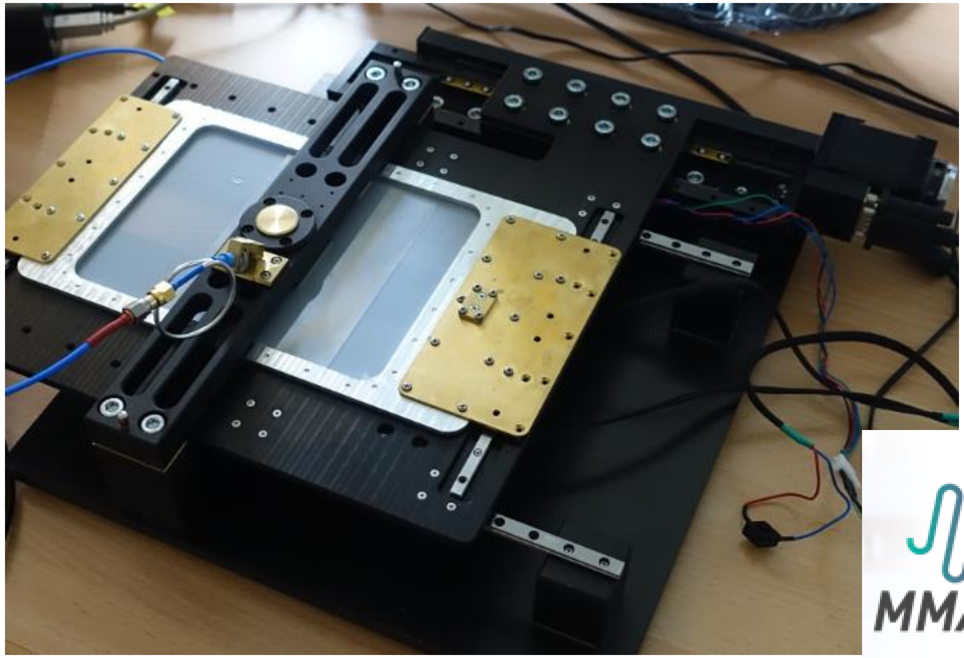
**Obviating the limitations:**

- *SUT thickness - slot size 0.6..6 mm* → *increase by decreasing frequency*
- **SUT lateral min size ("absolute" EM constraint) - 14..120 mm** → **scanning & postprocessing**
- **spatial resolution 14..120 mm** → **scanning & postprocessing**
- **SUT lateral max size – 40..150 mm** → **increase by change of mechanical construction**

**manual scanner for large panes of glass**
**(MW oven window)**



**automatic scanner**
**semiconductor wafers, composites, organic samples**

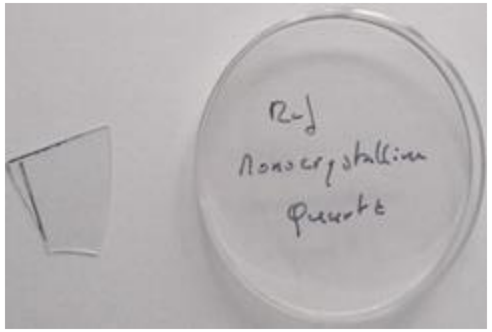


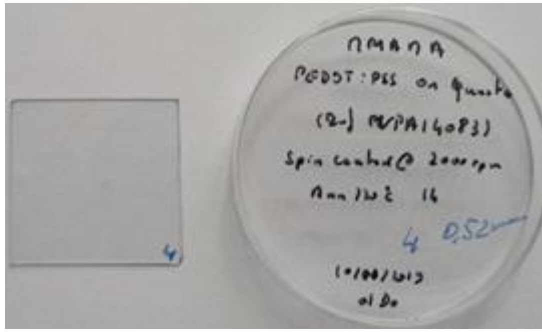
MMAMA

# Automatic surface scanning with SPDR

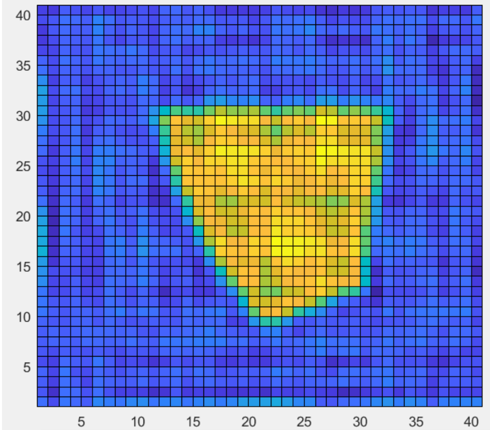

working with QWED Q-Meter

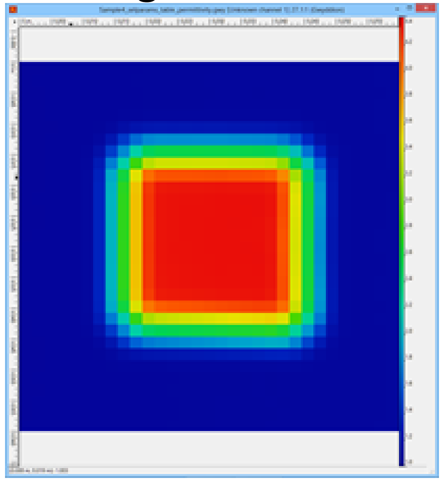
working with FieldFox
(Keysight hand-held VNA)

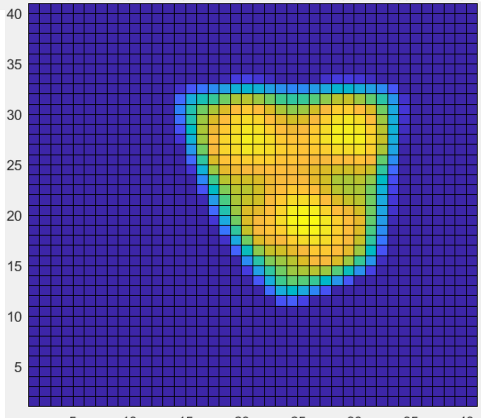




**samples from MateriaNova**
quartz substrate & deposited organic material



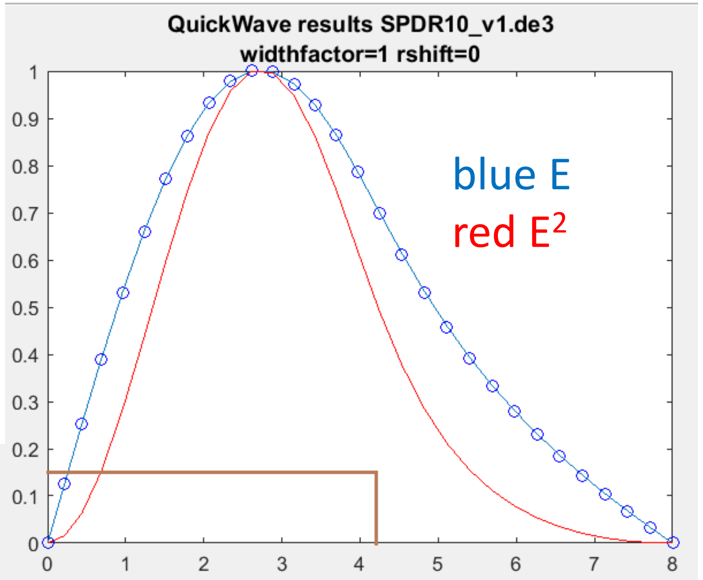


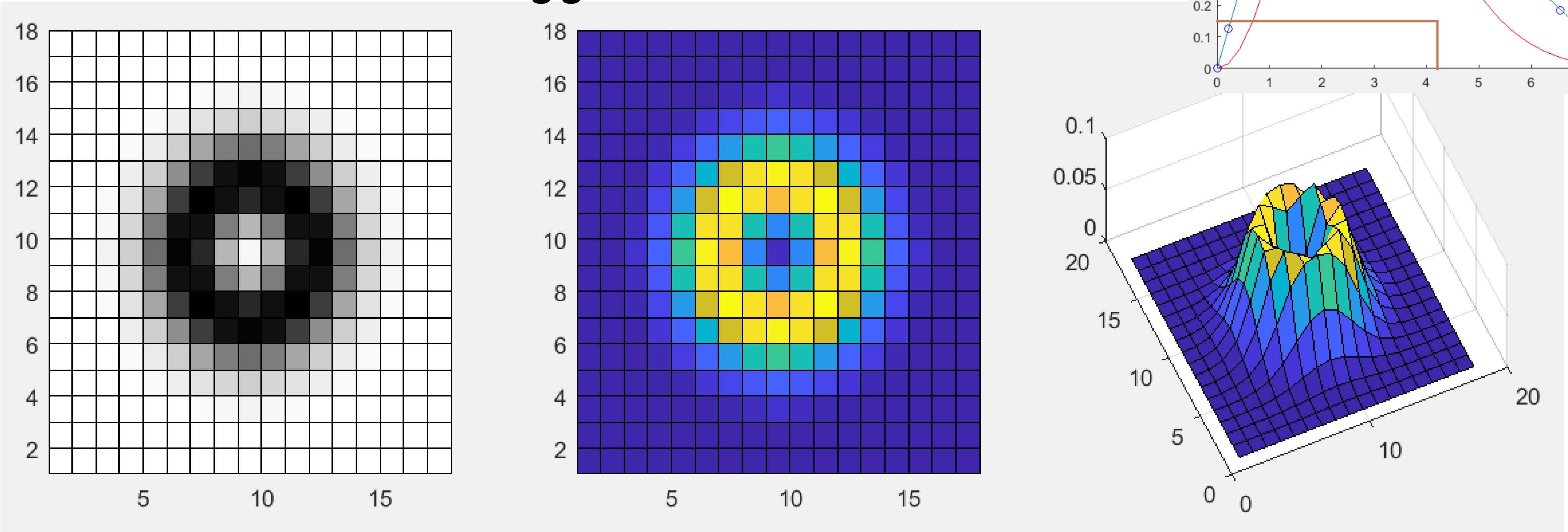

**scanning step 1mm**
**but resolution ~16mm !**
***→ seek modelling-based resolution enhancement***

# Resolution enhancement for SPDR imaging

**→ Parameters are "averaged" within DR head but we know the field pattern**

**E-field in our 10 GHz SPDR as simulated in QuickWave and tranferred onto the scanning grid:**



# Resolution enhancement for SPDR imaging

Consider the head meshed into $(2K+1) \times (2L+1)$ cells whose center with $E_T(0,0)$ is placed at cell $(m,n)$ the scan. For clarity, assume that the mesh is equidistant of raster $a$ ($a$ = 1mm in Fig. 1).
The measured energy change due to the SUT is:

$$\Delta W_{mn} = \frac{a^2 h}{2} \sum_{k=-K}^{K} \sum_{l=-L}^{L} \left[ \varepsilon_s^{'}(m+k, n+l) - 1 \right] E_T^2(k,l)$$

Arranging the 2D array of $\Delta W_{mn}$ into a 1D vector $W$ of elements $\Delta W_i$, $i=(n-1)*M+m$, $i=1,..,M*N$, and similarly the 2D array of permittivities $p_{s,mn}=(\varepsilon_s'-1)_{mn}$ into vector $P$:

$$[W] = [T]\,[P]$$

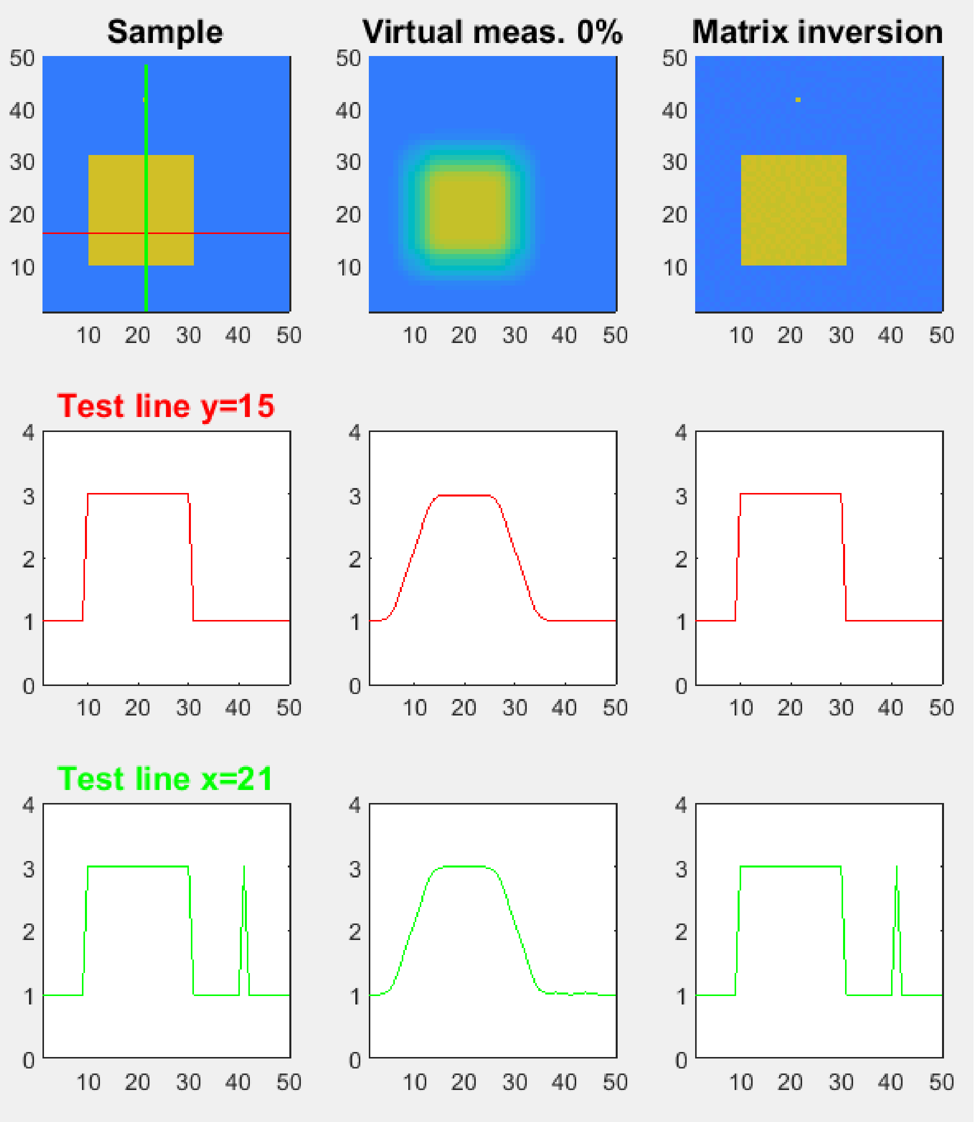
Matrix T is generated in such a way that element $t_{rs}$ in row $r$ and column $s$ is equal to :
- $|E_T(k, l)|^2$ for $s= r+k+M\,l$ for $k=-K..+K$ and $l=-L...+L$)
- 0 for $s$ not obeying the above condition.

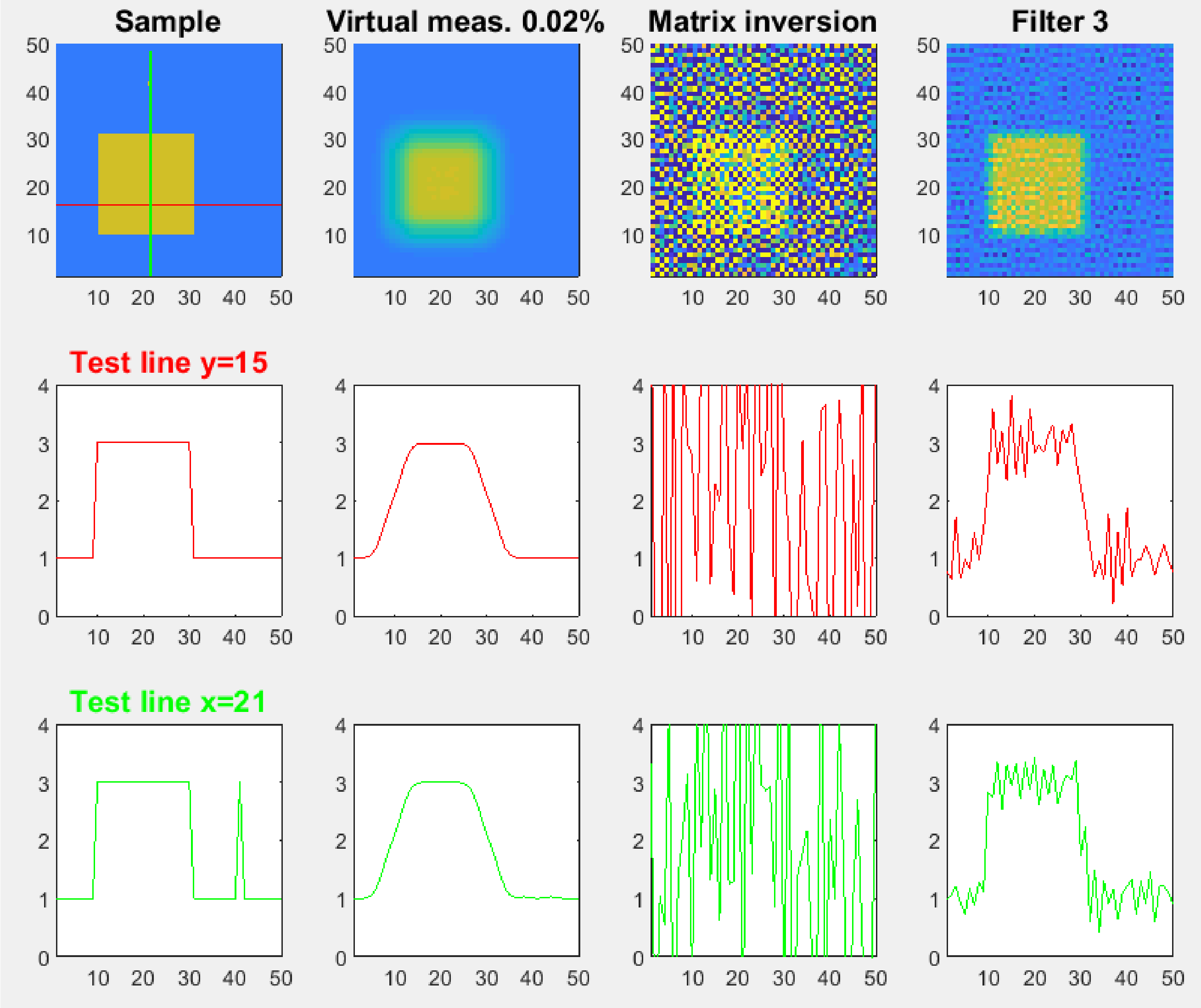
$$[P] = [T]^{-1}\,[W]$$

**Space-domain,**
***not* Fourier - domain**

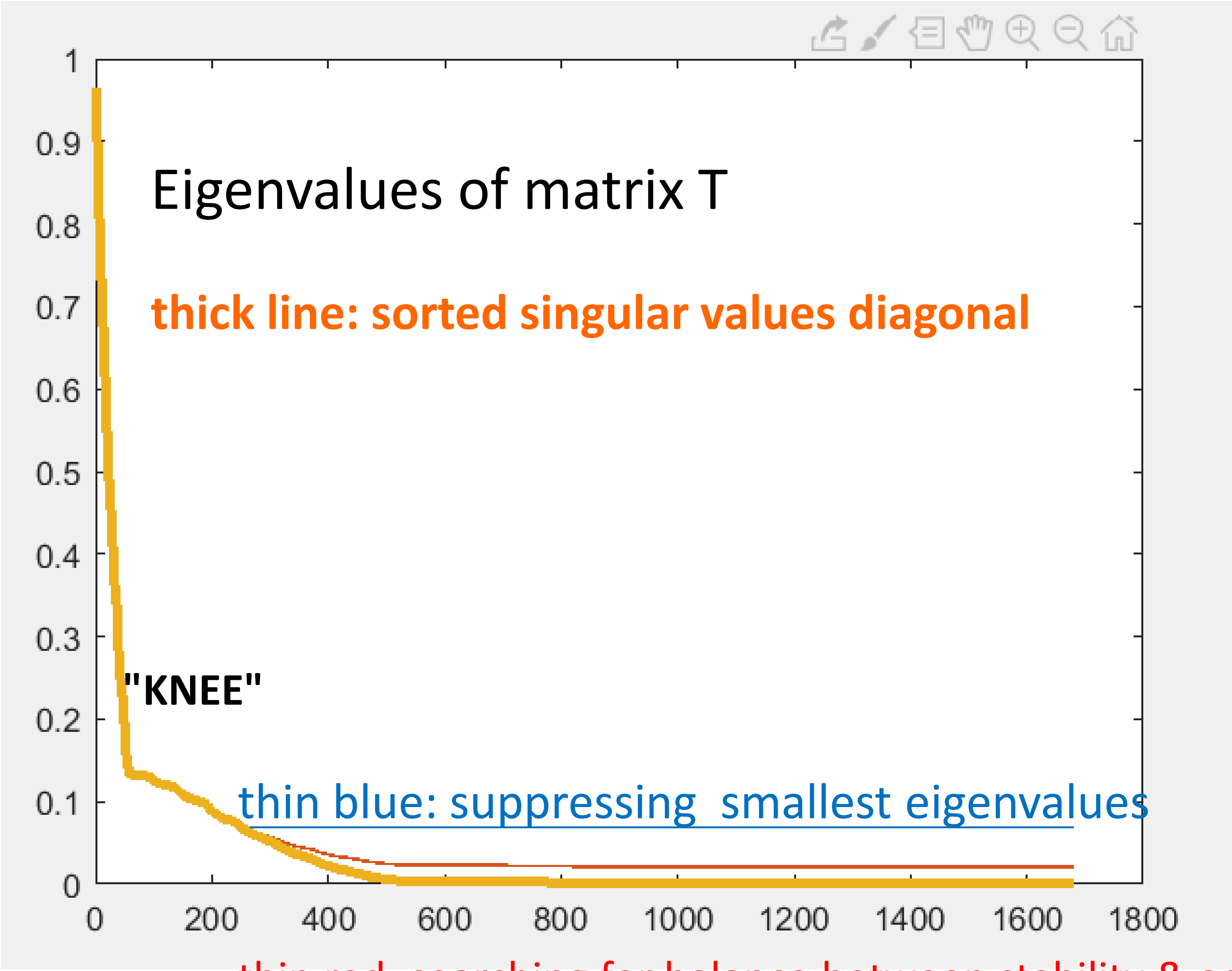
Matrix $T$ is large, $M*N \times M*N$, but sparse and has a banded structure.

# MATLAB experiments with virtual scans: matrix inversion of exact data & with noise

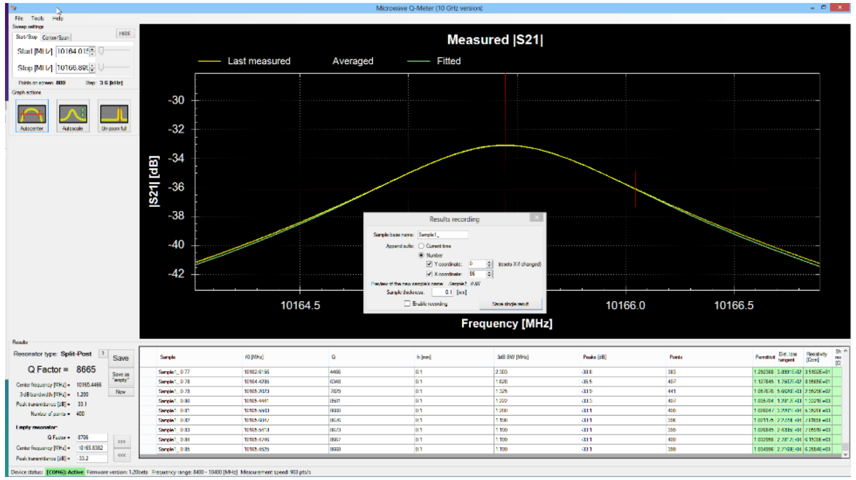


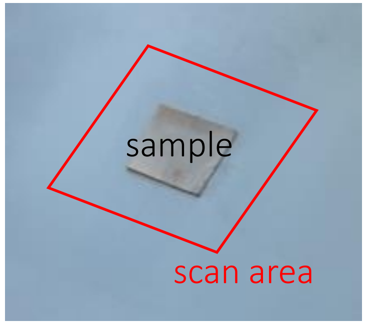
# Singular Value Decomposition

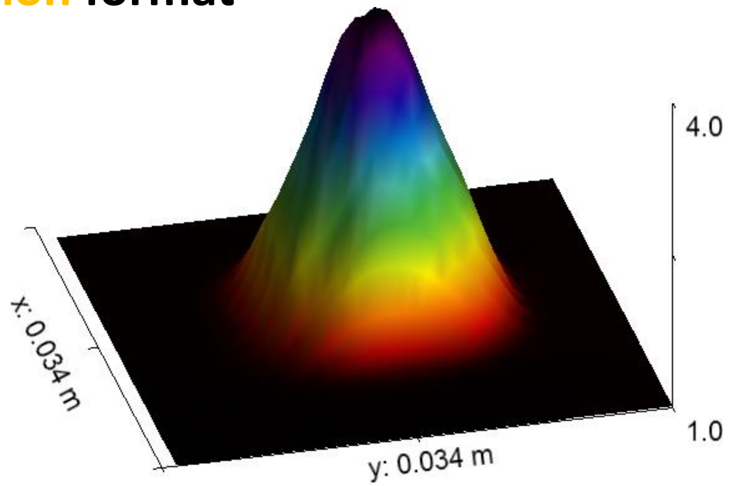



thin red: searching for balance between stability & accuracy

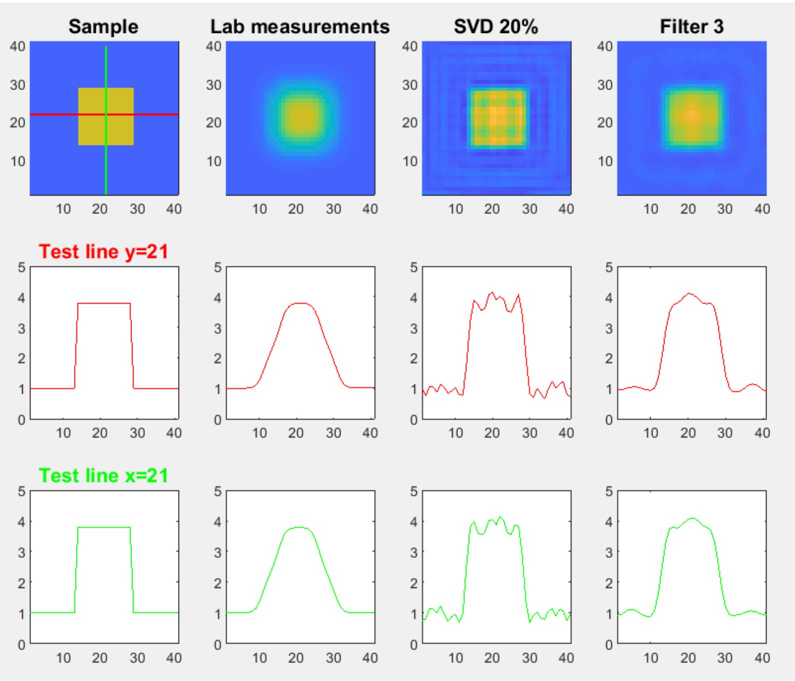


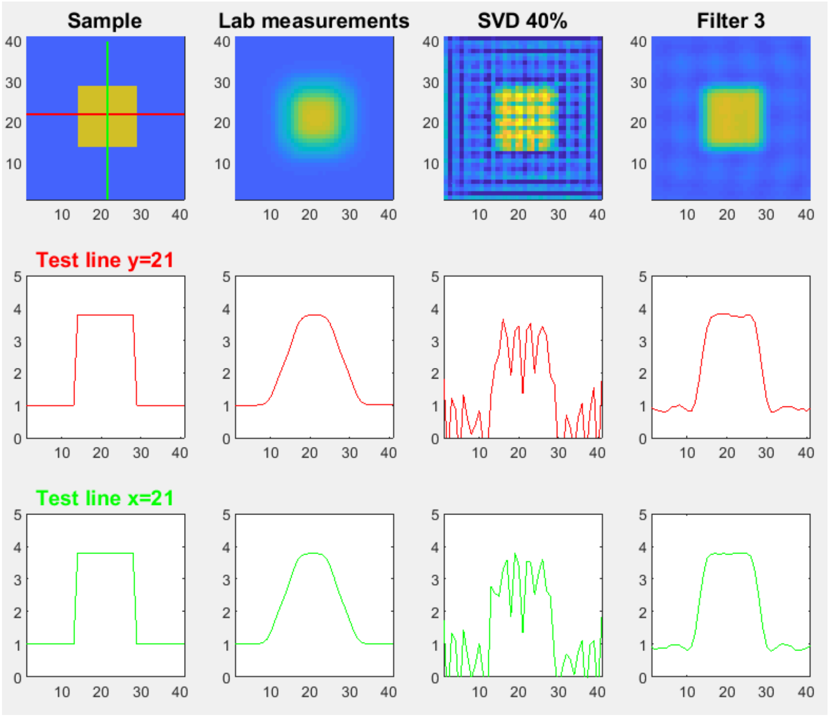

**scan area 41x41mm**
**=> matrix 1681x1681 (step 1mm)**
**SUT laminate Rogers R4003 h=20mils (0.508 mm)**
**SUT size 15x15 mm**
**scan saved in Gwyddion format**

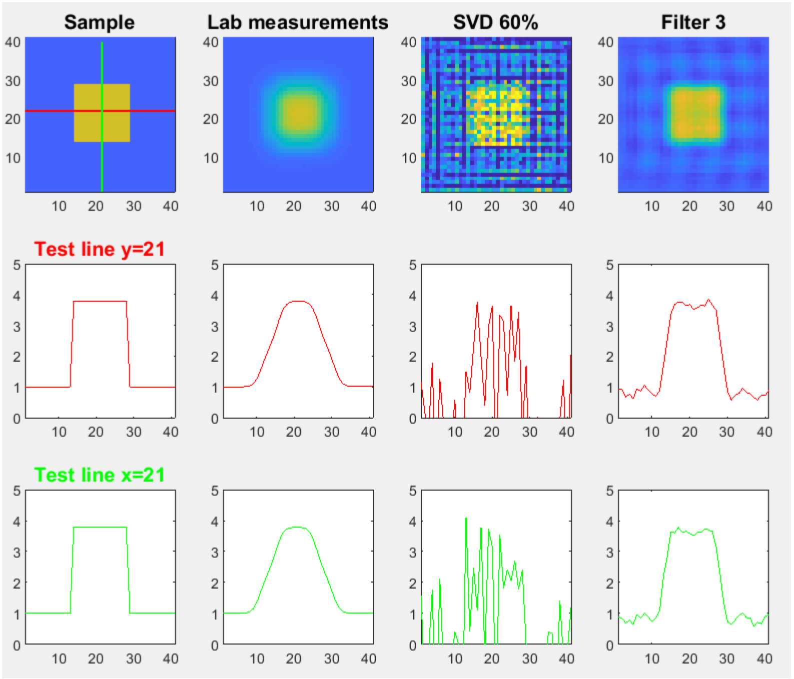


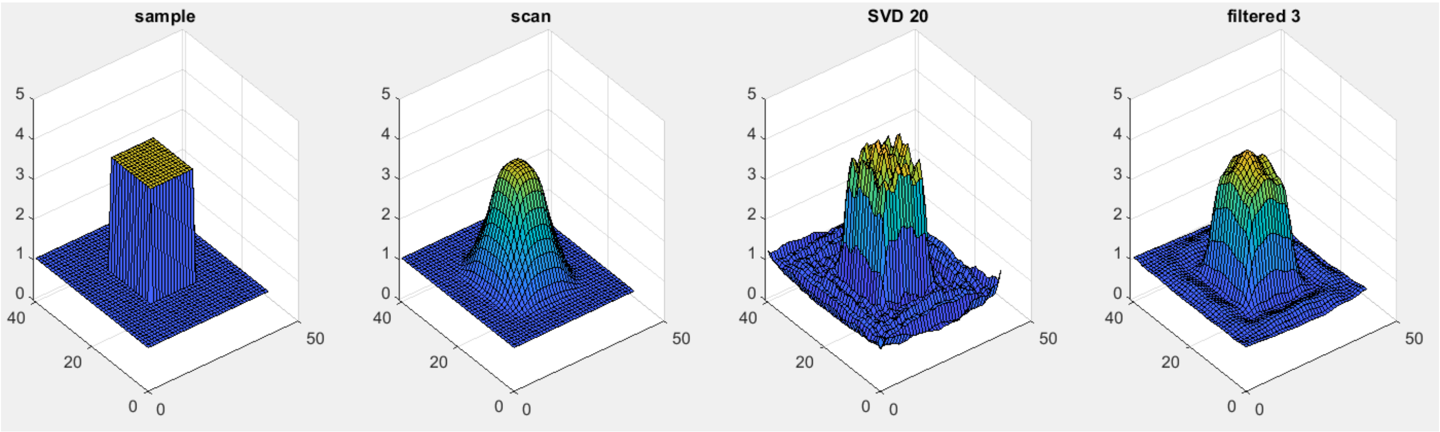



# MATLAB experiments with laboratory scans: experimenting with SVD parameters



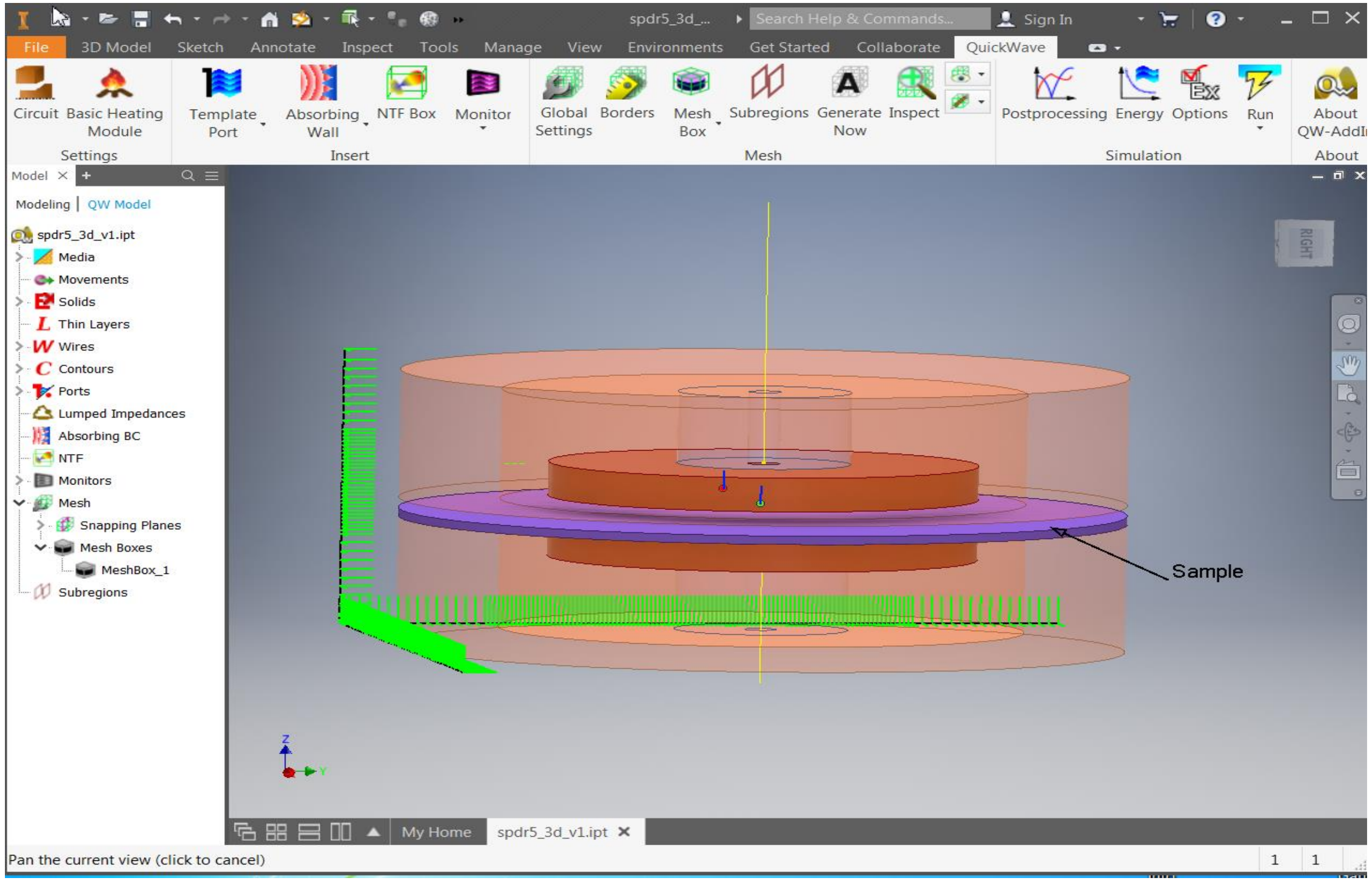



# Modelling validation of SPDR method assumptions

**How much is the E-field pattern influenced by SUT?**

**→ application of "*near field imaging*" in QuickWave**



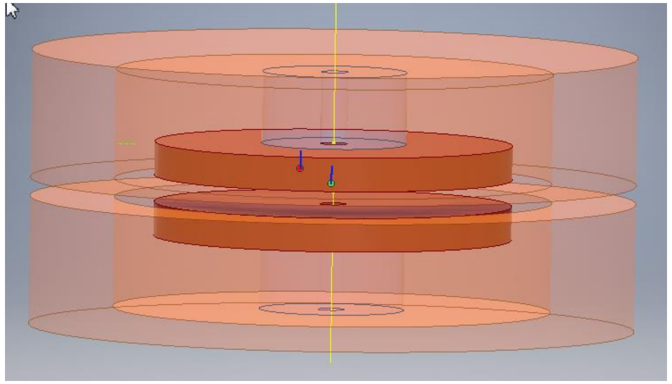

**10 GHz SPDR model in QW-AddIn for Autodesk® Inventor® Software (common environment for modelling & manufacturing)**

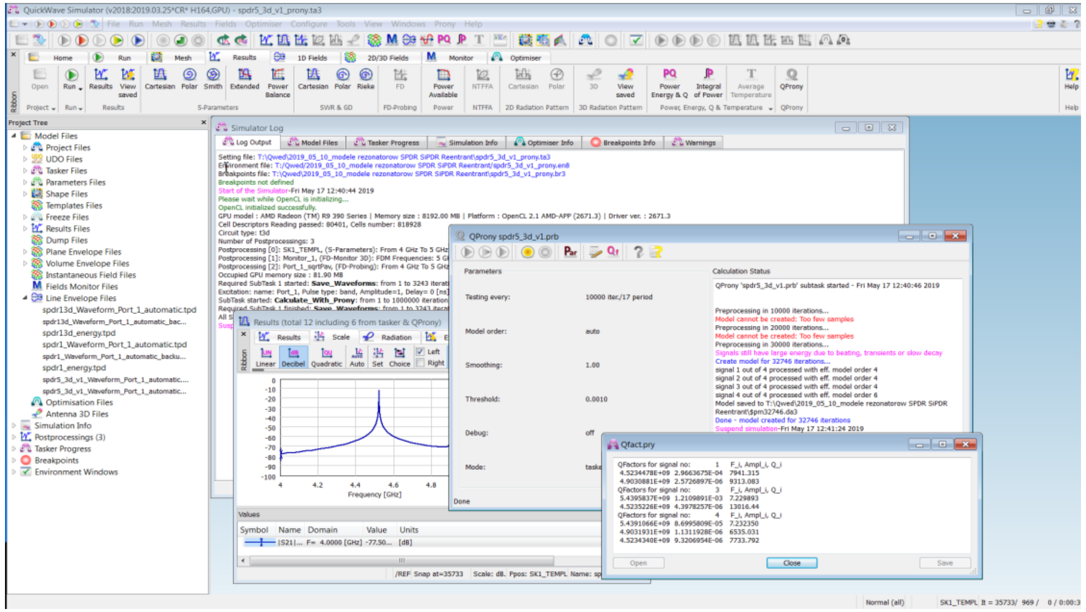
# Modelling validation of SPDR method assumptions

**How much is the E-field pattern influenced by SUT?**

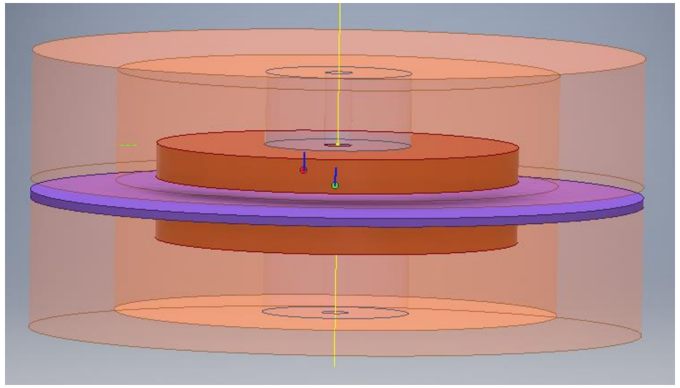
**→ application of "*near field imaging*" in QuickWave**

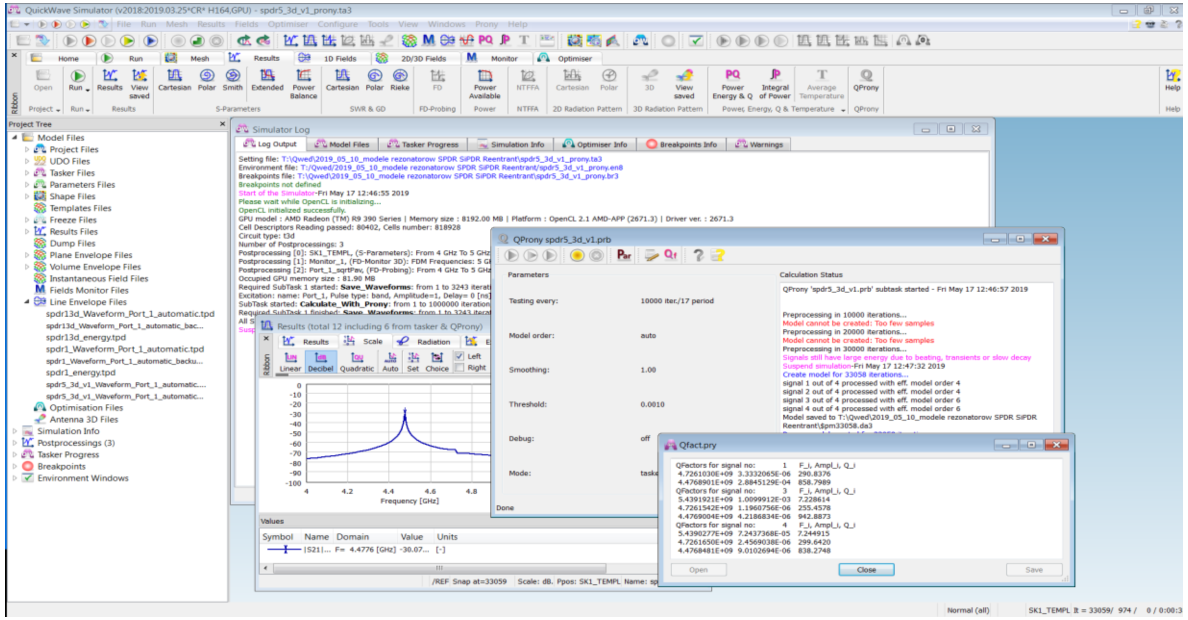
**empty**





**with SUT**

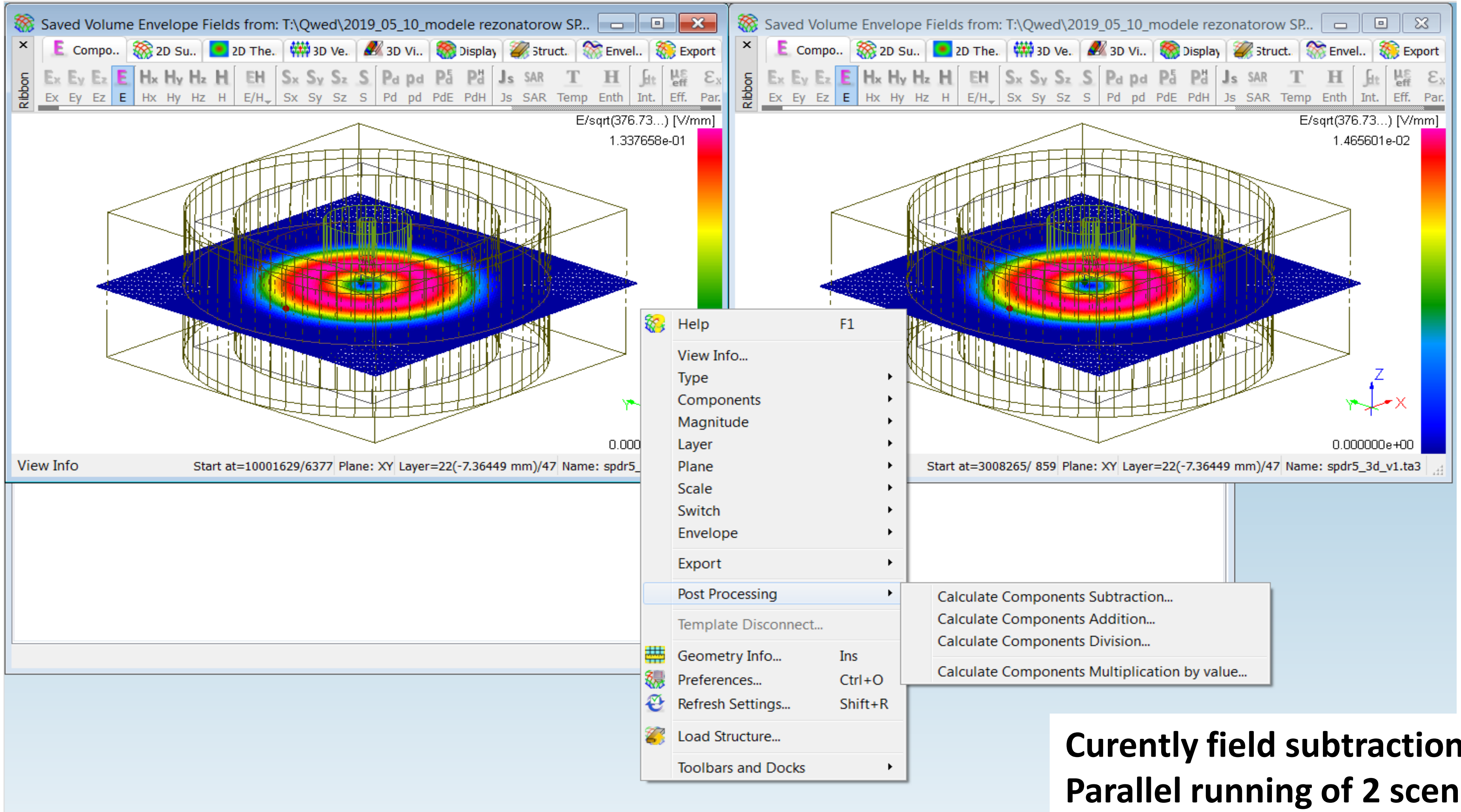




# Modelling validation of SPDR method assumptions

**How much is the E-field pattern influenced by SUT?**

**→ application of "*near field imaging*" in QuickWave**

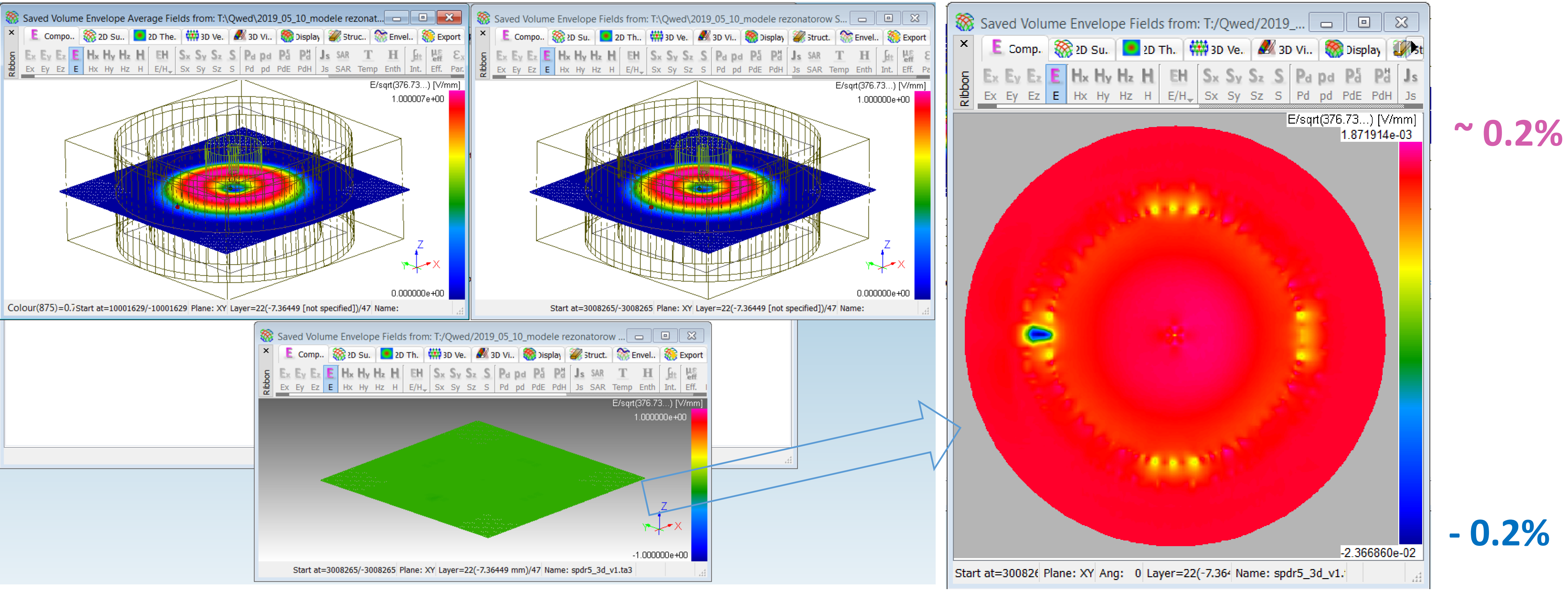



**Curently field subtraction performed on saved fields.**
**Parallel running of 2 scenarios under development.**

# Modelling validation of SPDR method assumptions

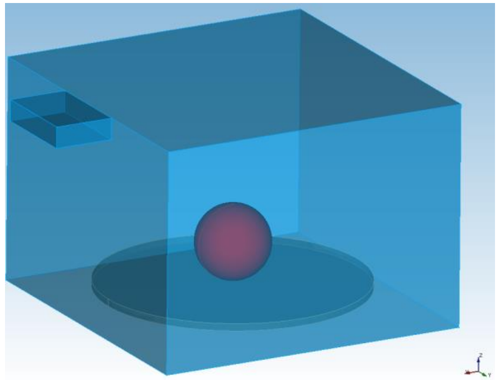
**How much is the E-field pattern influenced by SUT?**

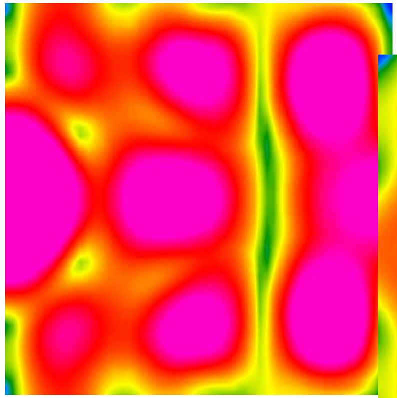
**→ application of "*near field imaging*" in QuickWave**



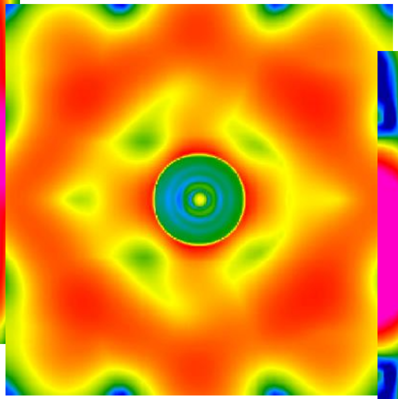
# Advanced near-field imaging functionality

**Separation of incident and diffracted fields (*option implemented per request of P.O.Risman, Malardalen Univesity*)**

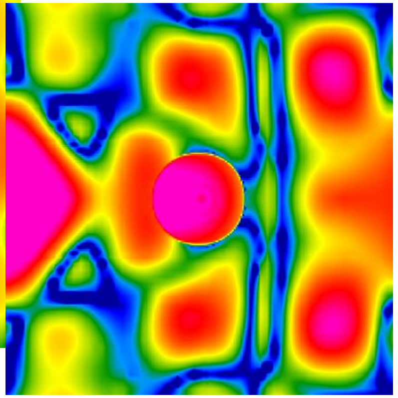




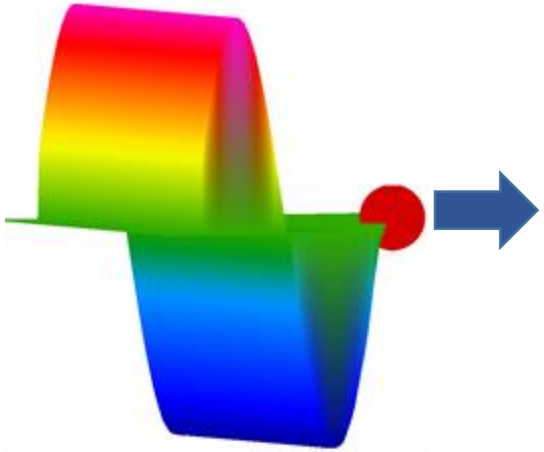
E-field in an empty cavity

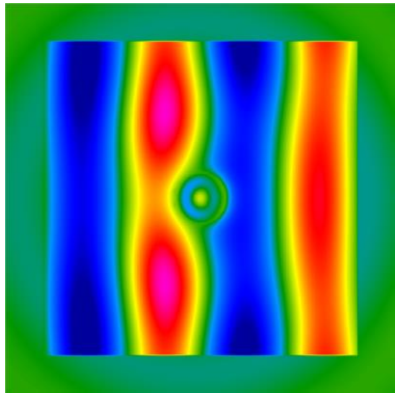


E-field in a loaded cavity

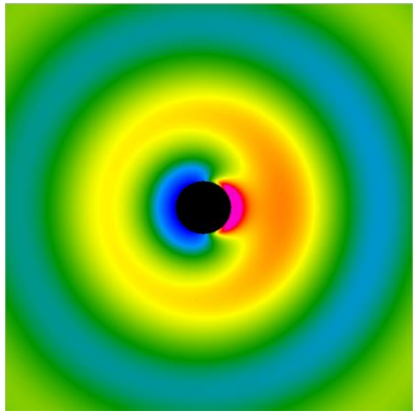


Scattered near-filed in cavity



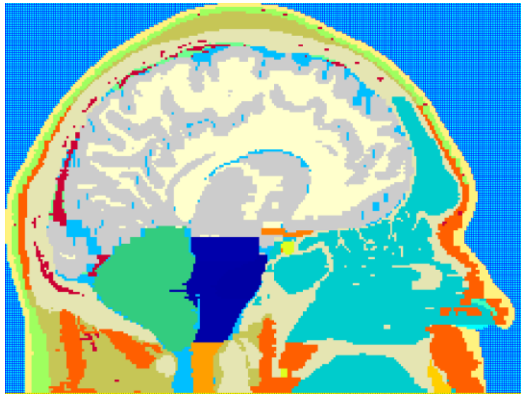


Total field
Focusing by the load
„exploding egg effect”

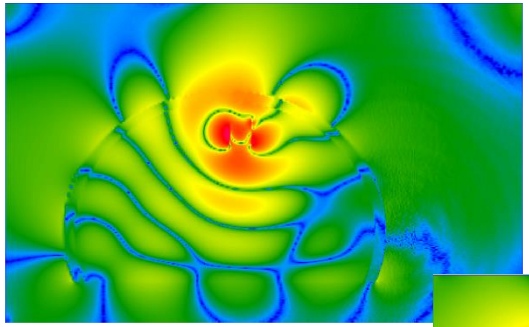


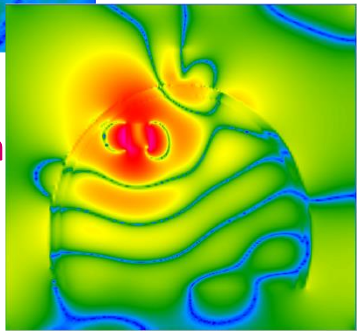
Diffracted field reveals cause of focusing: circumferential resonance

**Detection of inhomogenities in tissues**



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





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

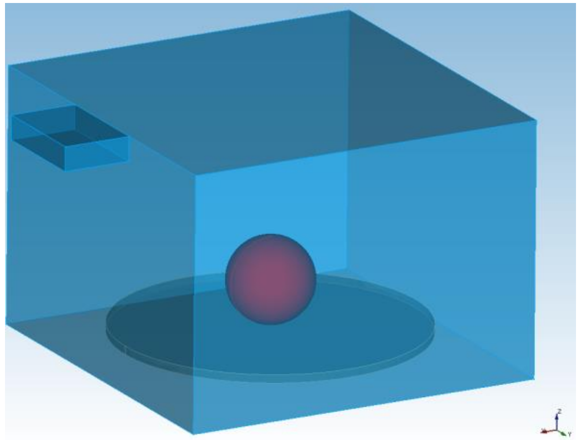


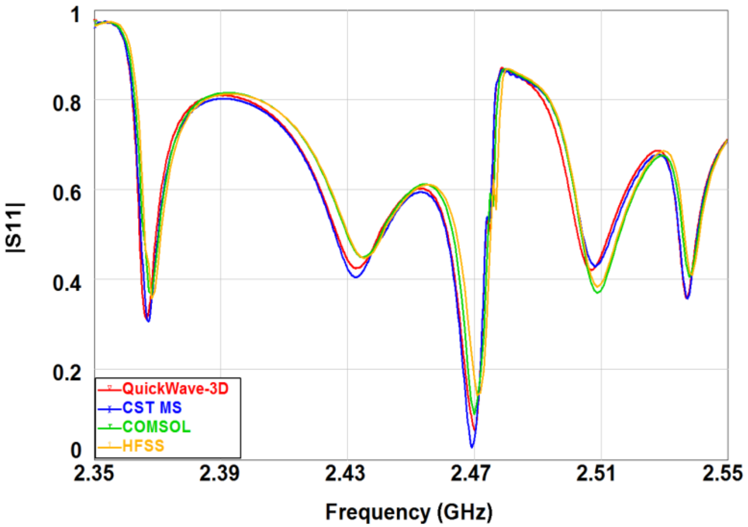
* https://sites.utexas.edu/austinmanaustinwomanmodels/

# Accurate modelling of coupled electromagnetic-thermal problems

## Application to microwave processing of materials

**Simple microwave heating benchmarks & microwave heating phenomena studies***



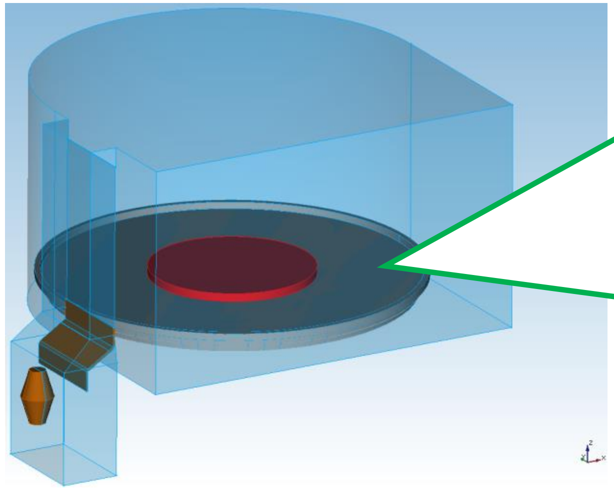



- heat transfer & load dynamics
- Load rotation & arbitrary movement during heating
- Source parameters tuning – regime for solid state sources
- Thermal dependence of materials
- Fluid Flow

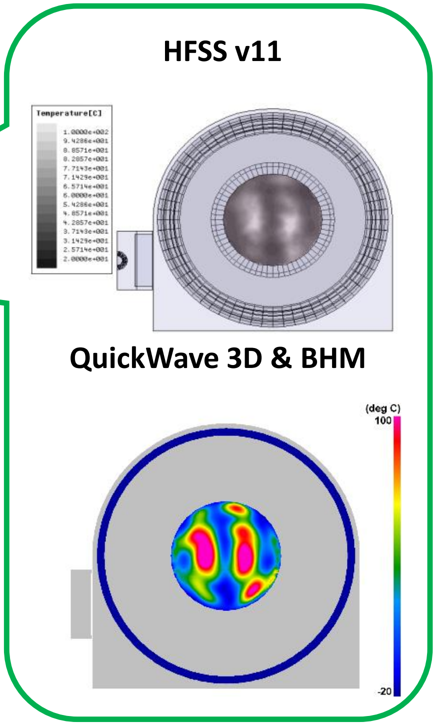
**Freezing to file the state of the simulation**

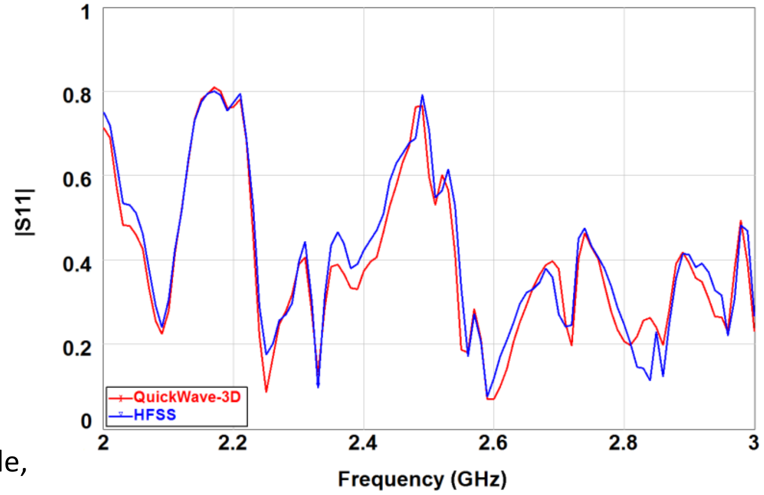
**De-freezing on arbitrary computer & at convenient time**

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



Courtesy of Whirlpool Inc. – Whirlpool MAX oven

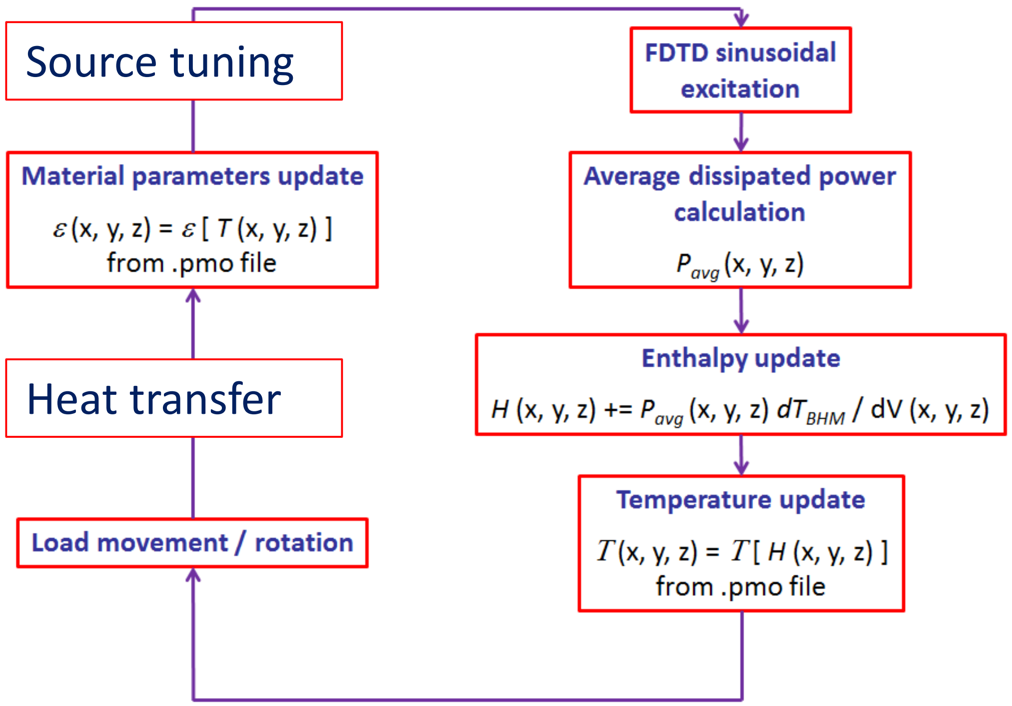


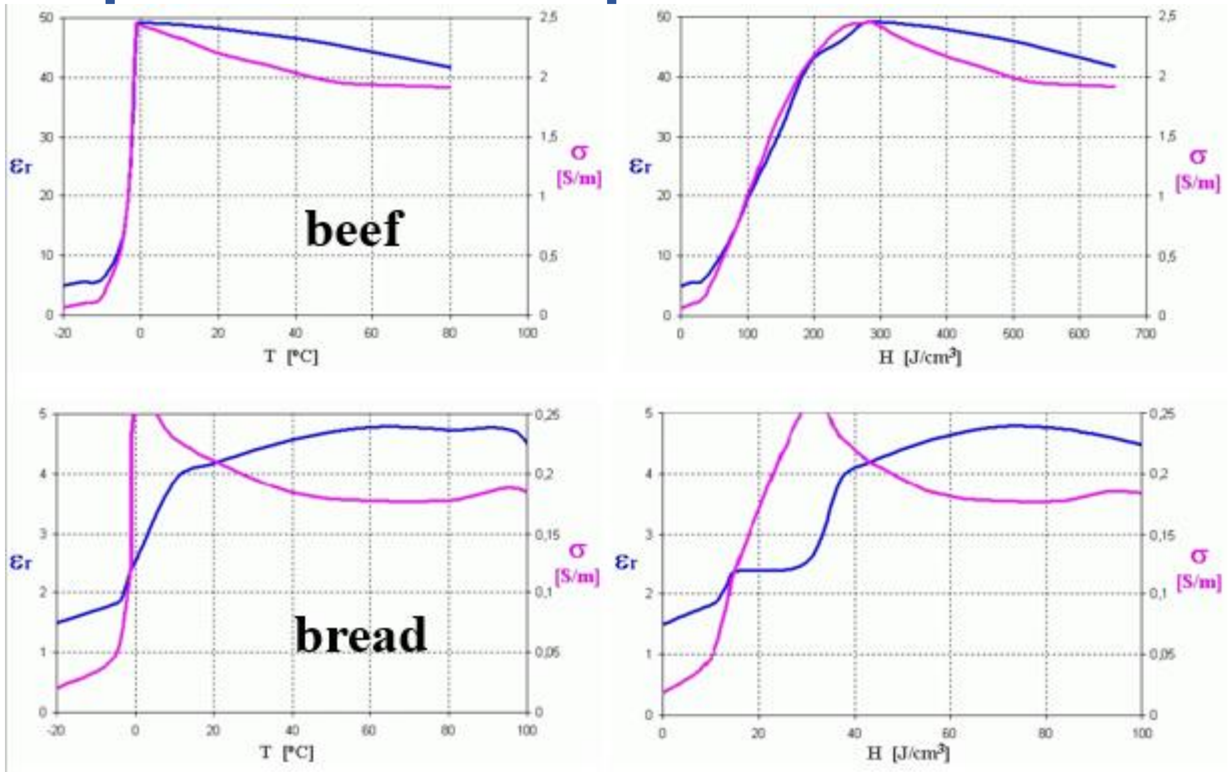



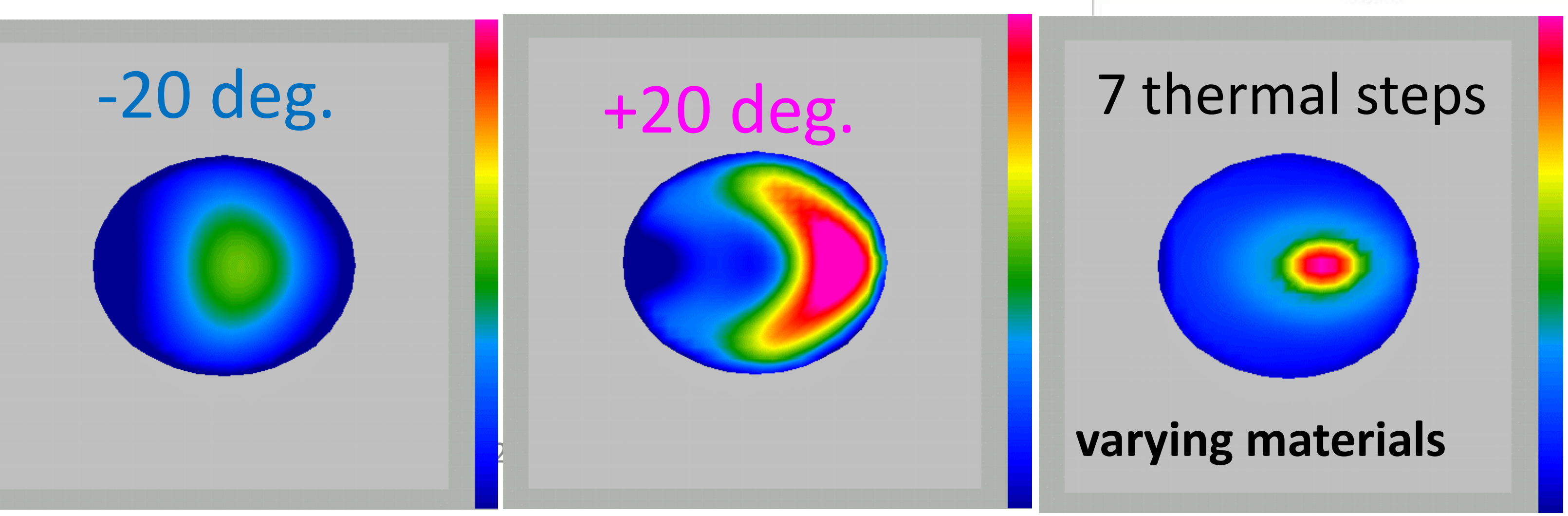

With QuickWave EM computation as fast as 1 min 18s on a low-cost video card – supporting all graphic cards with OpenCL

* 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.

# Multiphysics modelling: temperature-dependent materials



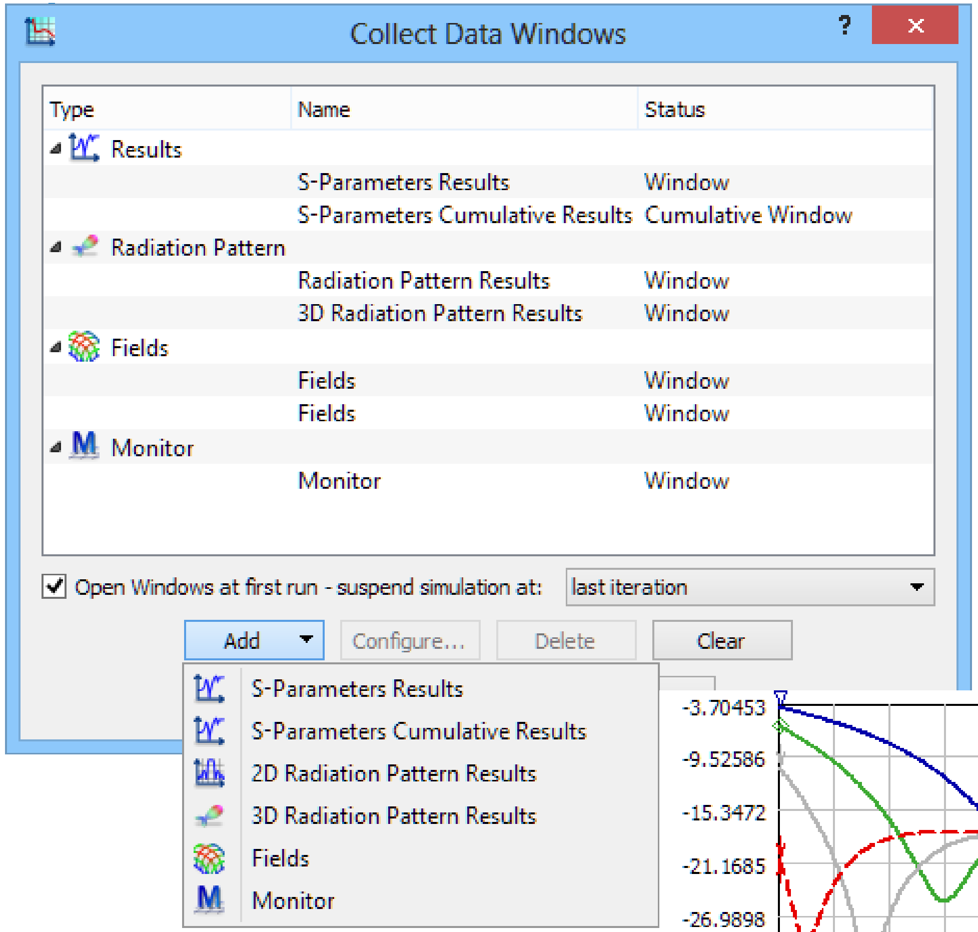



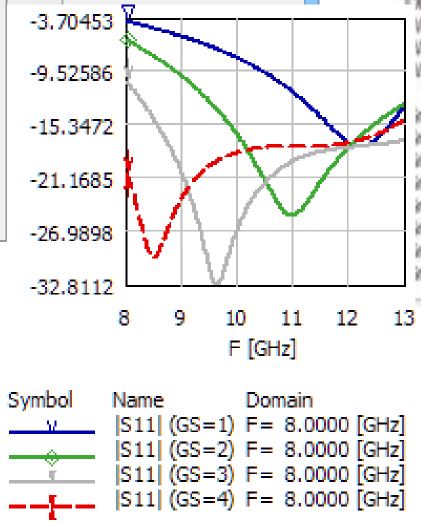

**QW-BHM module of QuickWave:**

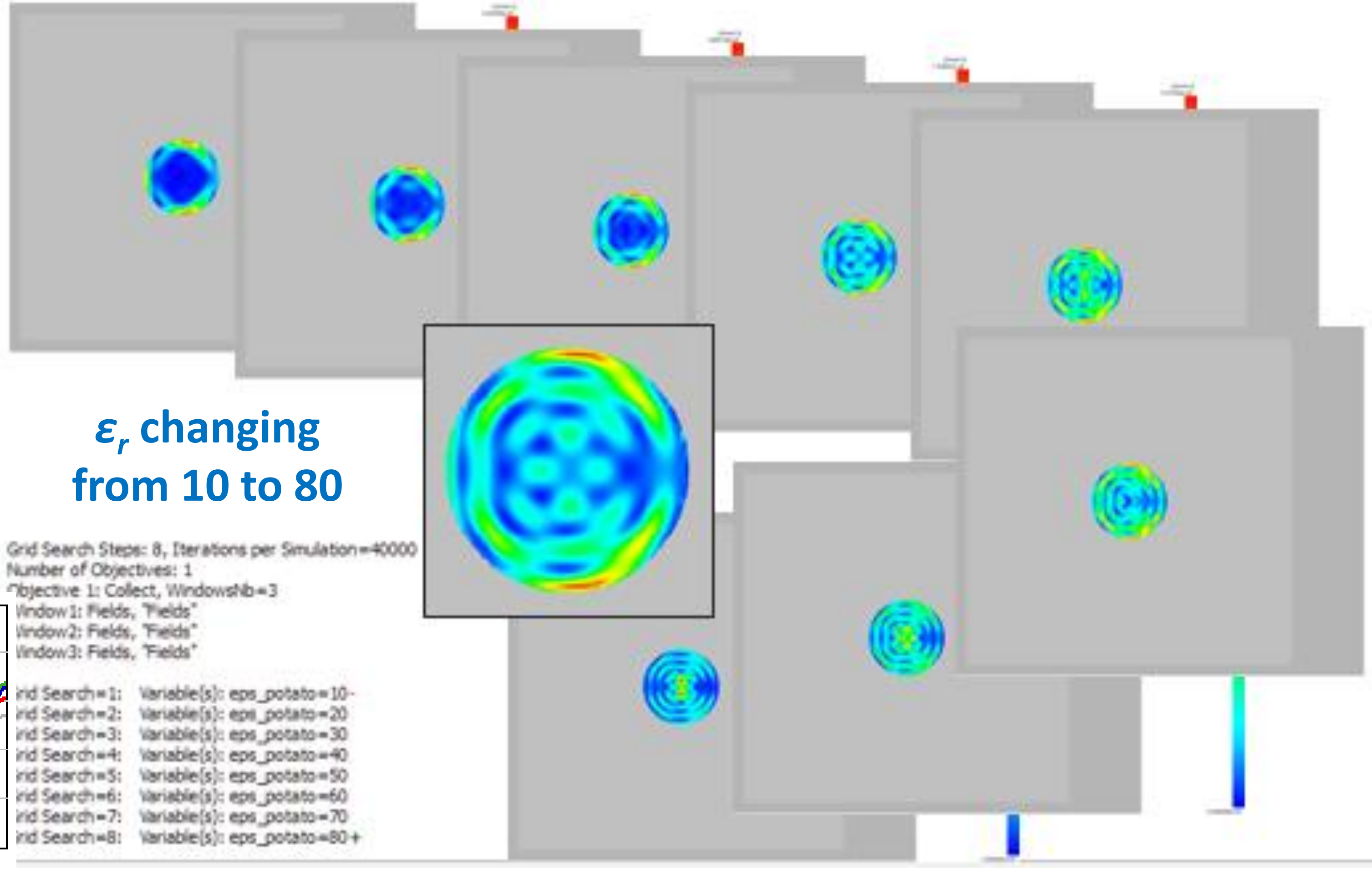
- **automatic system**
- **each cell heated individually**
- **no need to define 1000s of "media"**
- **bilateral coupling EM - thermal**

# Multiphysics modelling: *Collect Data* in *Grid Search*

***Collect Data*** **of S11 and dissipated power density in potato heated in MW oven, as text files and GUI**




**$\varepsilon_r$ changing from 10 to 80**

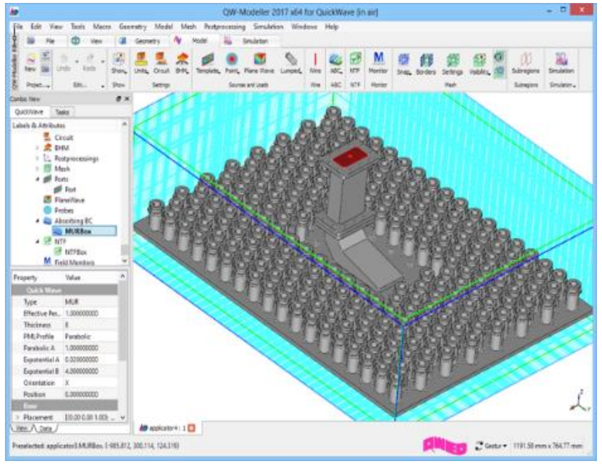
**Note: automatic multiple switching from pulse to sine excitation implemented in QuickWave for matching source to load.**

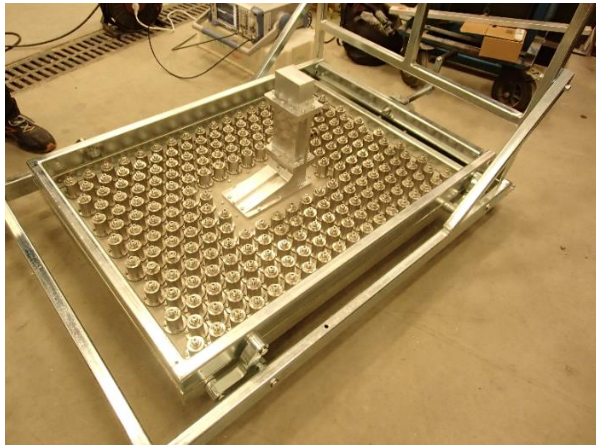
# Unusual QuickWave applications

## High power applicator for µW treatment of bituminous surfaces aiming at road repair

**Challenges**

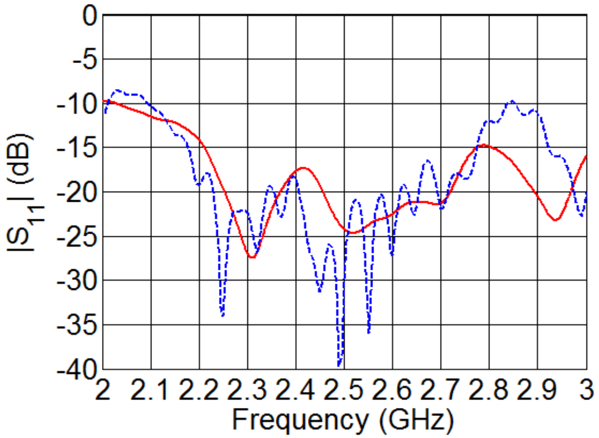
- High dissipation of µW power in road surface
- Safety issues – prevention of EM energy leakage



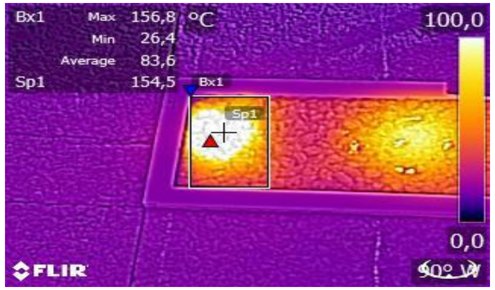


High power applicator with a system of chokes preventing µW energy leakage

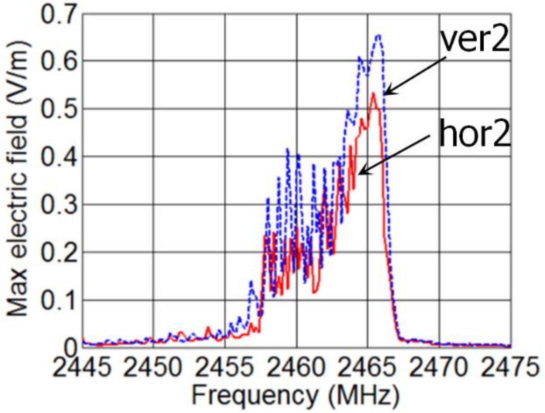
**Simulated & measured reflection coefficient**



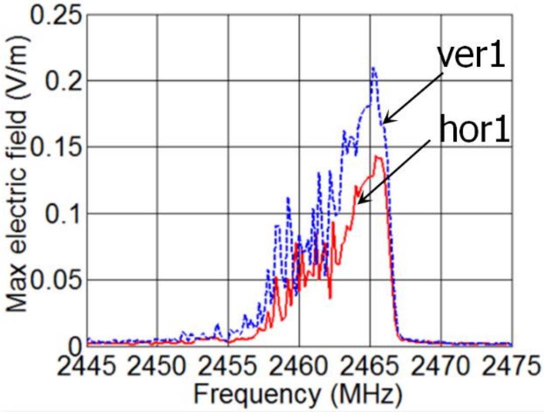

**Measured temperature distribution**



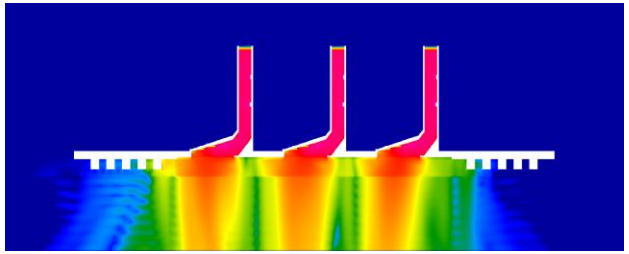

**Exposure levels @ 0.5m from applicator Below standardized limits**

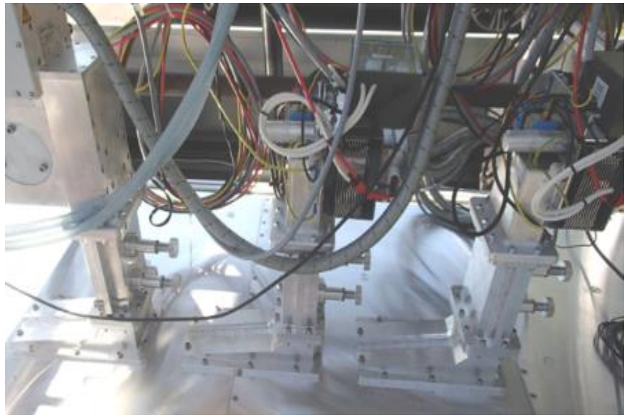



**On a side**




**In front**

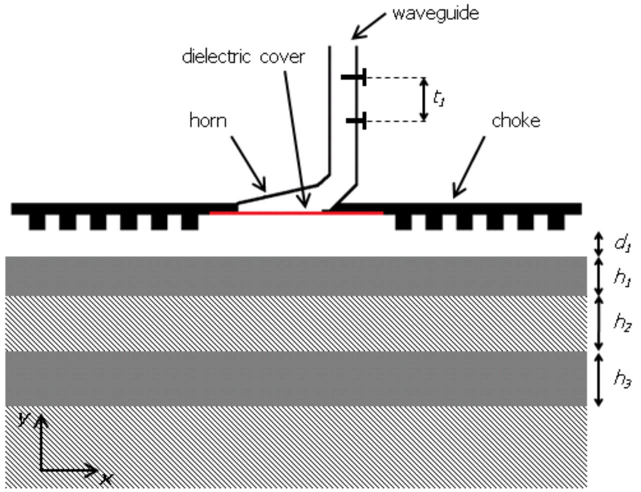


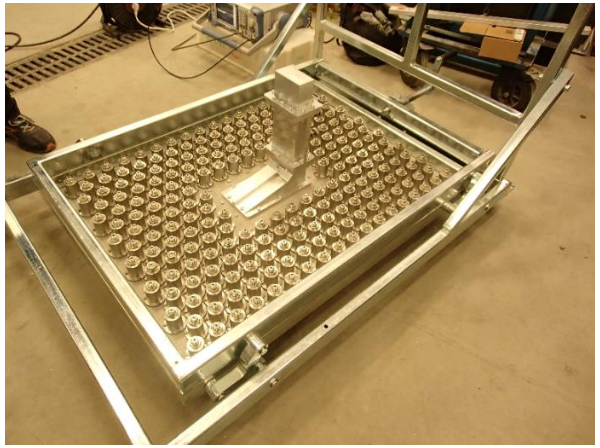


System of three MW power applicators with feeding system and leakage preventing chokes: designed, manufactured, tested


B. Salski, M. Olszewska-Placha, T. Karpisz, J. Rudnicki, W. Gwarek, M. Maliszewski, A. Zofka, J. Skulski, "Microwave applicator for thermal treatment of bituminous surfaces", *IEEE MTT Trans.*, vol. 65, no. 99, pp. 1-9, 2017

# Advanced optimisation and parameters sweep workflows



Microwave applicator for thermal treatment of bituminous surfaces

B.Salski et al., *IEEE MTT Trans.*, vol.65, Sep.2017.

Internal optimisation

Optimisation with external tools – commercial and in-house

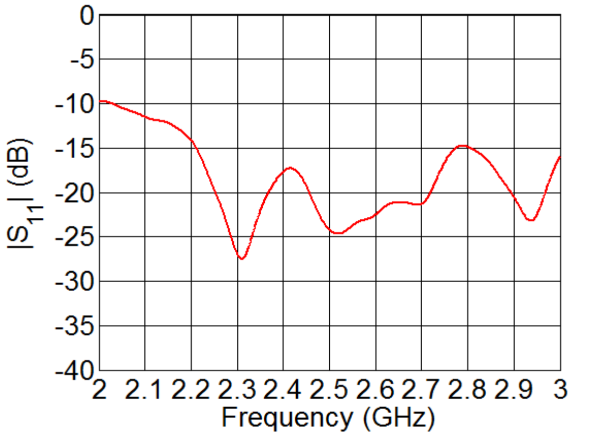
Typical, software predefined optimization objectives, e.g. S-parameters, Radiation patterns (incl. fit under user-defined radiation envelope), etc.

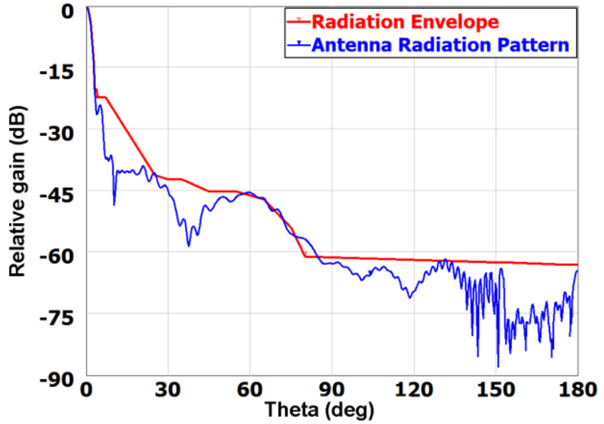
All simulation available objectives, e.g. power dissipated, shielding effectiveness, radiation efficiency, etc., through external data-extraction application

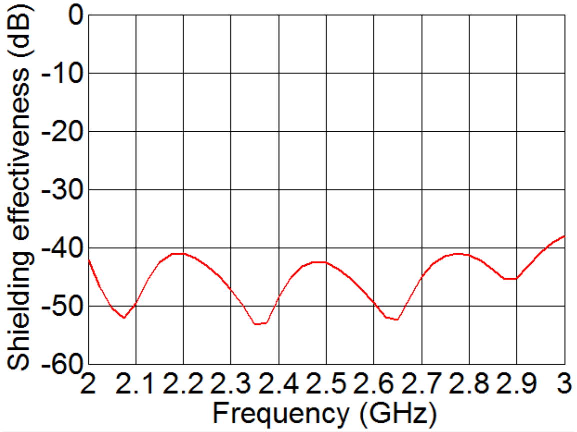
Simulation results saved to file

External application – objective extraction from file

Optimiser – internal or external

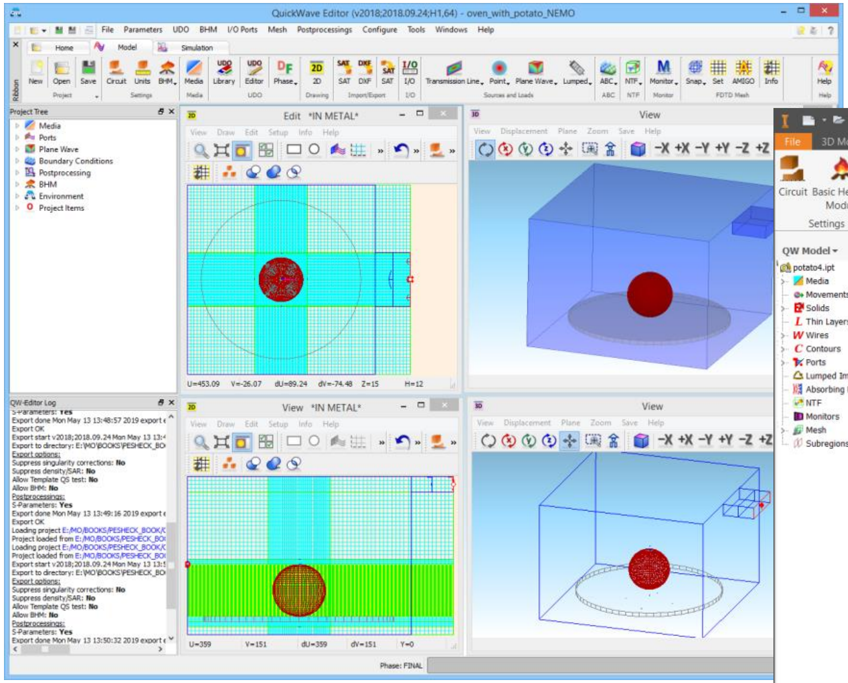


# Dedicated user interfaces for parametrised project creation

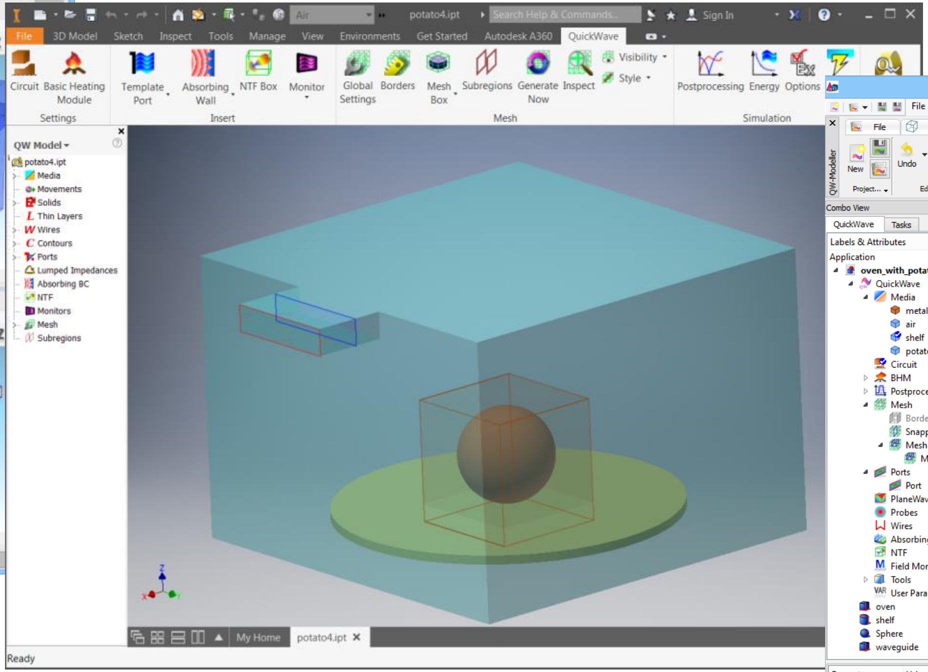
## QW-Editor



**In-house, script based**

Import/export to *.sat & *.dxf

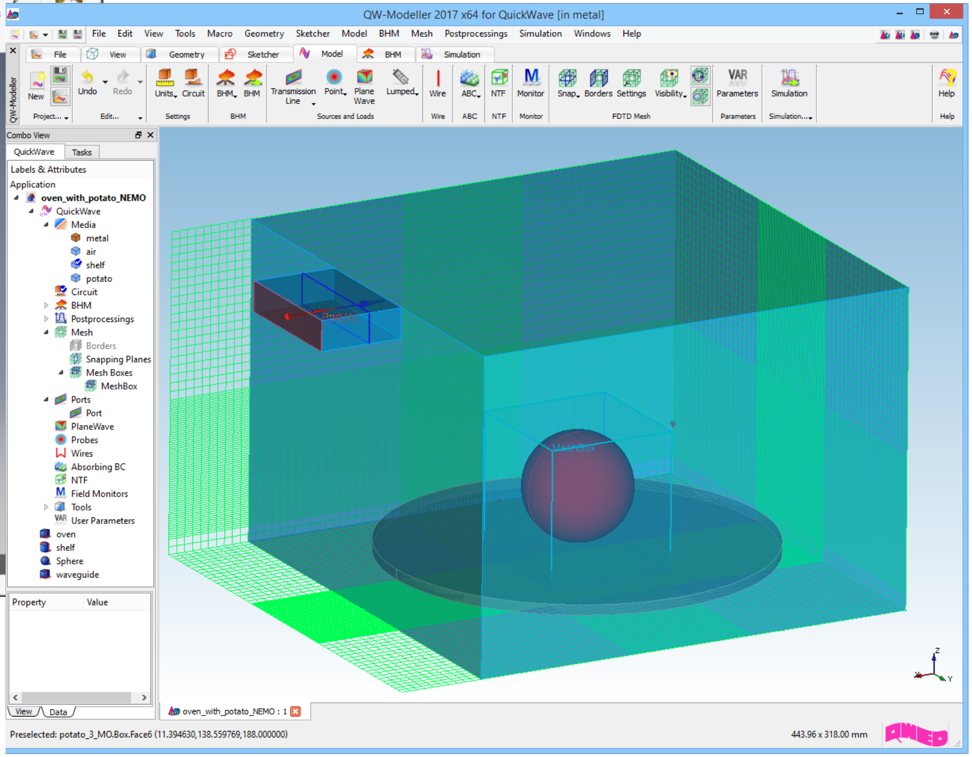
## QW-AddIn for Autodesk Inventor Software



**Based on advanced professional CAD tool**

**Import/export to e.g. *.sat & *.step**

## QW-Modeller



**CAD tool - FreeCAD based**

**Free of charge, No licences, No time restrictions, No project limitations**

**Import/export to e.g. *.step, *.iges & *.dxf**

***Curiosity: export of CAD files from "old" QW-Editor for further manufacturing is reported by our user.***

# Conclusions

**With this talk I seek collaborations:**

**on the development of:**

- **material measurement test-fixtures,**
- **applicators for processing of materials,**
- **software models & workflows for material modelling.**

**on behalf of:**

- **QWED team,**
- **our European projects MMAMA, NanoBat,**
- **members of broader EU initiatives, e.g. European Materials Modelling Council.**

# THANK YOU!