

***Modelling - based methodology  
for downscaling dielectric resonator  
material measurements of material surfaces***

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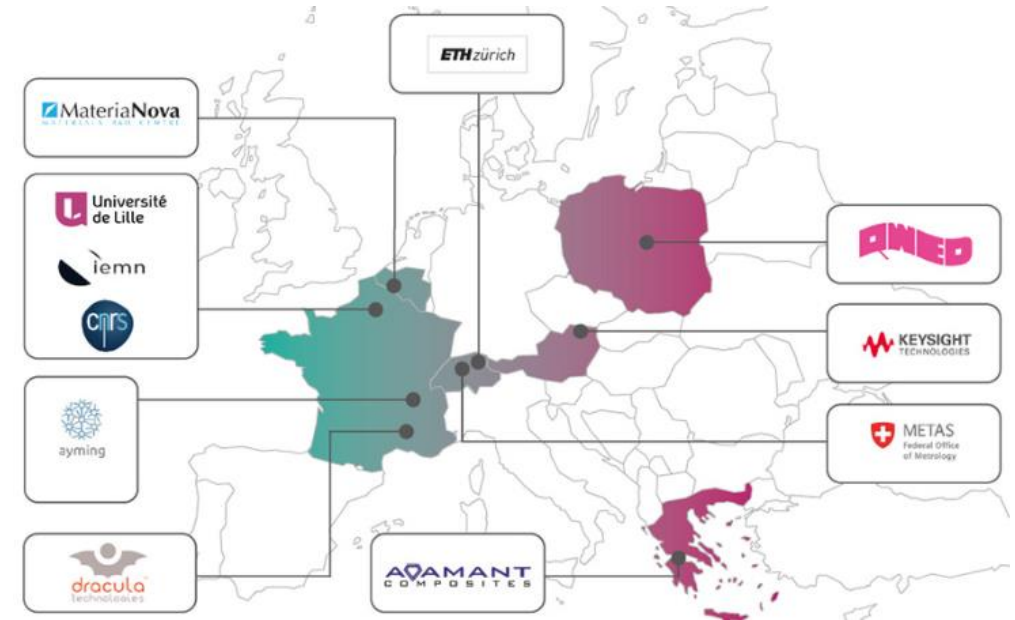
**→ *How we apply general-purpose EM software  
to enhanced material measurements & processing***

*with contributions from: M.Olszewska-Placha, M.Sypniewski, J.Rudnicki*



# Acknowledgements

The work presented has received funding from the  
*European Union's Horizon 2020*  
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 under grant agreement  
*MMAMA n°761036.*  
 (website: [www.mmama.eu](http://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 of material images**
- **"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  $\epsilon_s = \epsilon_s' - j \epsilon_s''$  is inserted into DR:  
 resonant frequency changes from  $f_e$  to  $f_s$   
 Q-factor changes from  $Q_e$  to  $Q_s$ .

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

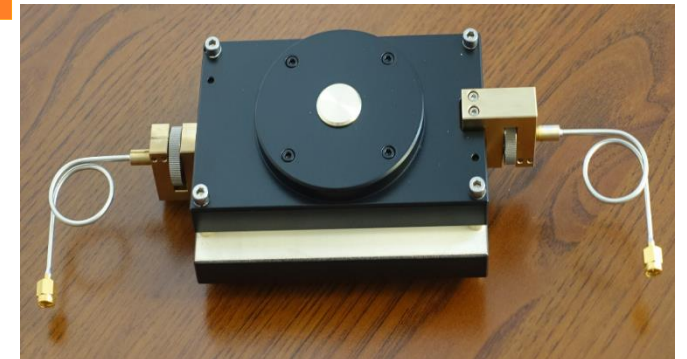
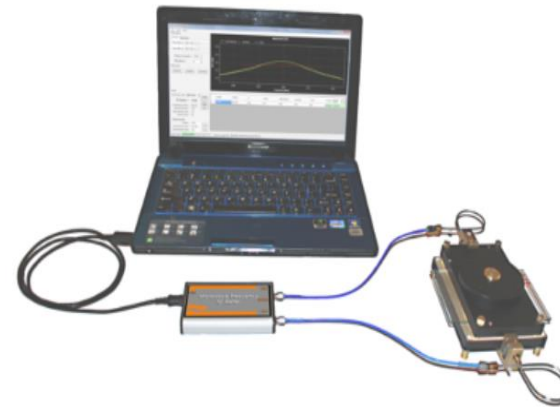
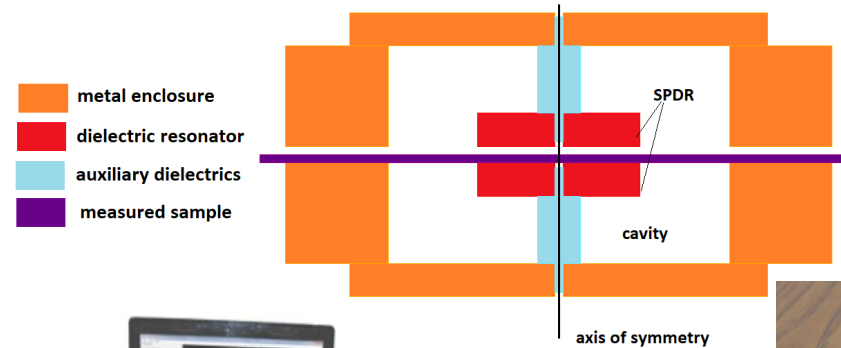
$$\frac{1}{Q_s} - \frac{1}{Q_e} \approx \frac{h}{C} \iint_S \epsilon_s''(x, y) E^2(x, y) dS$$

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

field assumed invariant in z-direction  
 S is called the DR's *head*

**sign**  $\approx$  reflects field pattern changes caused by SUT

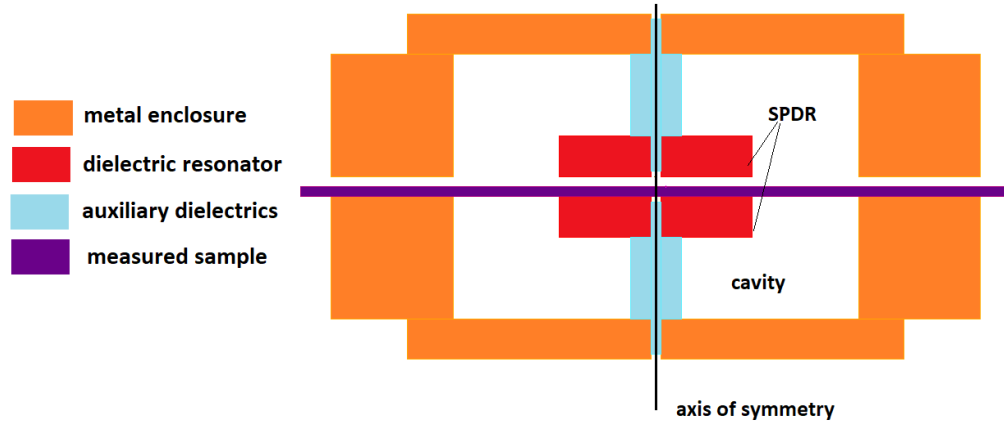
Most popular example: **Split-Post Dielectric Resonator**



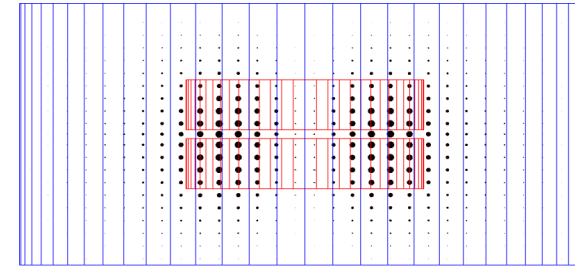
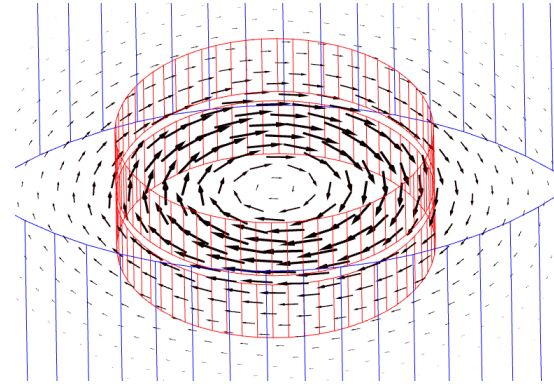
minimise

field variation in z (or take it into account)  
 field changes due to SUT

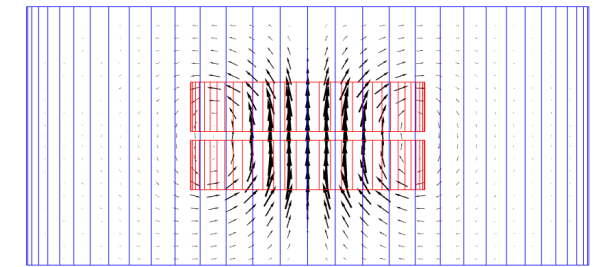
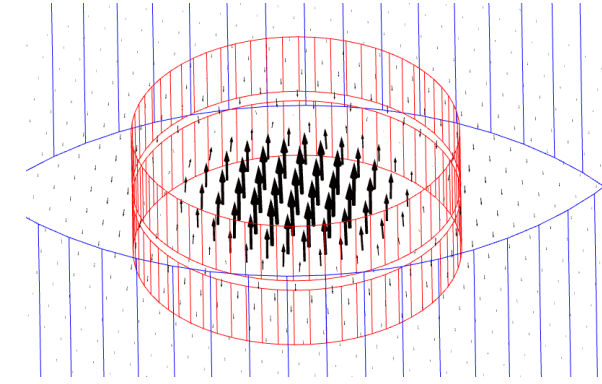
# Fields in SPDR



## E-field



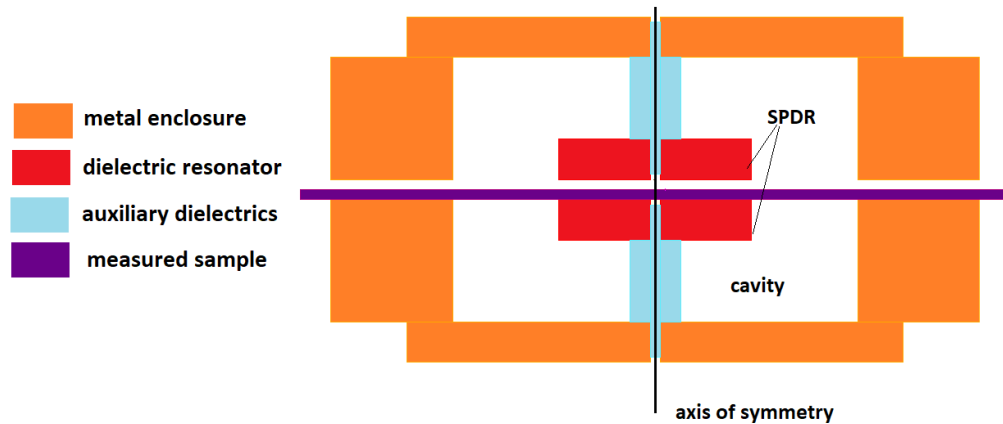
## H-field



- resonant mode with EM fields mostly confined in and between those ceramic posts → **minimal 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 is 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

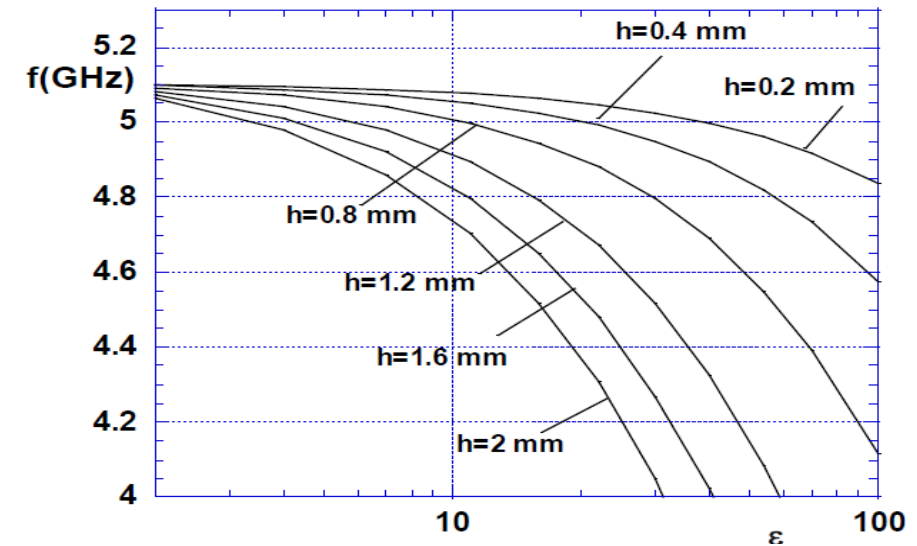


accuracy for  $\epsilon$  typically 0.3%  
measurable losses  $\tan\delta \sim 6 \cdot 10^{-5}$

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

## Limitations:

- 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



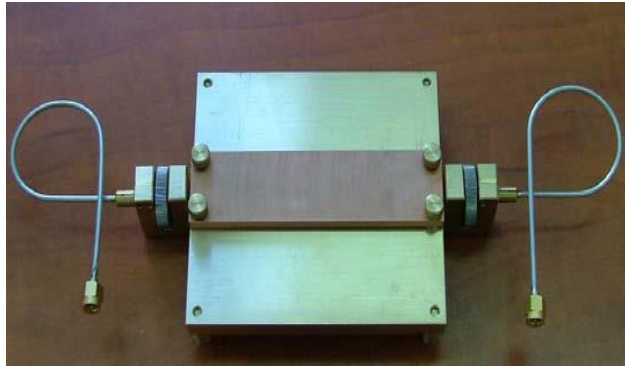
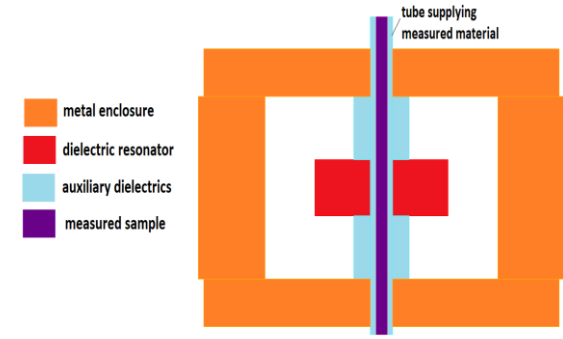
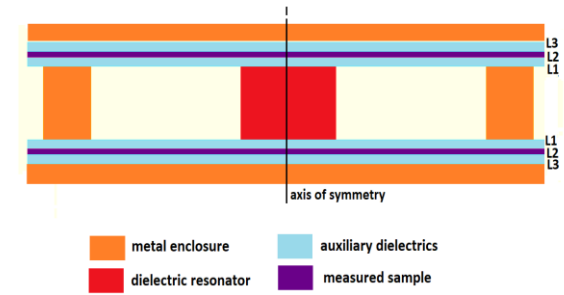
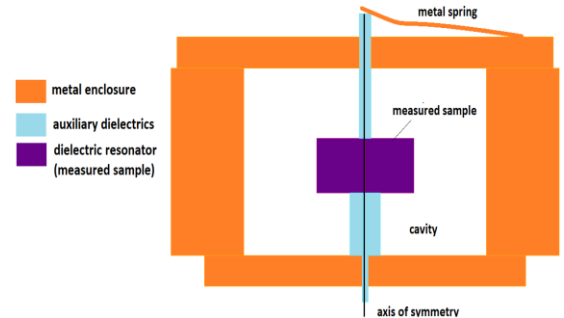
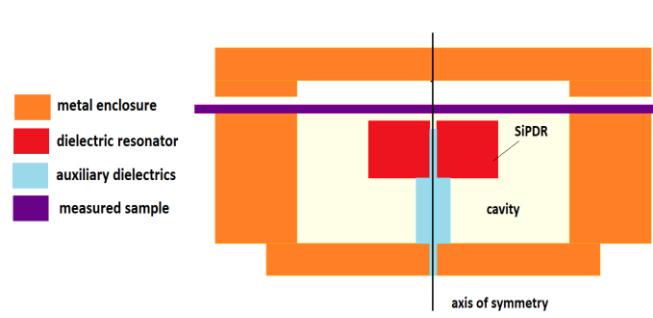
$$\Delta\epsilon/\epsilon = \pm(0.0015 + \Delta h/h)$$

$$\Delta\tan\delta = \pm 2 \cdot 10^{-5} \text{ or } \pm 0.03 \cdot \tan\delta \text{ whichever is higher}$$

	Conductivity [1/( $\Omega\text{m}$ )]	Resistivity [ $\Omega\text{ cm}$ ]	Surface resistivity [ $\Omega/\text{sq}$ ]
Range of SPDR applications	from $10^{-2}$ to 1	from $10^2$ to $10^4$	from $5 \cdot 10^3$ to $10^6$
Range of SiPDR applications	from 1 to $10^7$	from $10^{-5}$ to $10^2$	from $2 \cdot 10^{-4}$ to $5 \cdot 10^3$
Sapphire	$> 5 \cdot 10^6$		



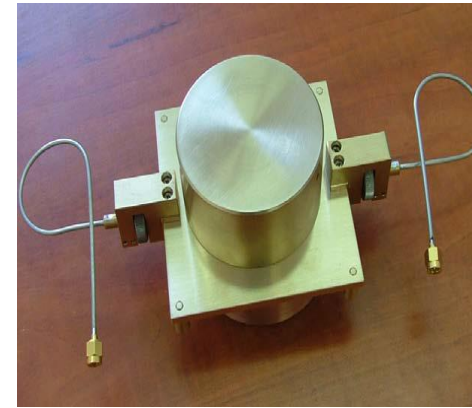
# Other types of dielectric resonators (TE<sub>01δ</sub>)



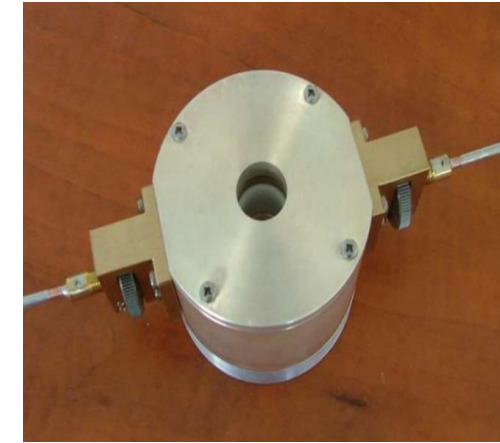
single-post  
resistive sheets



cavity  
resonating SUT  
ultra-low-loss SUTs



sapphire  
metal SUTs



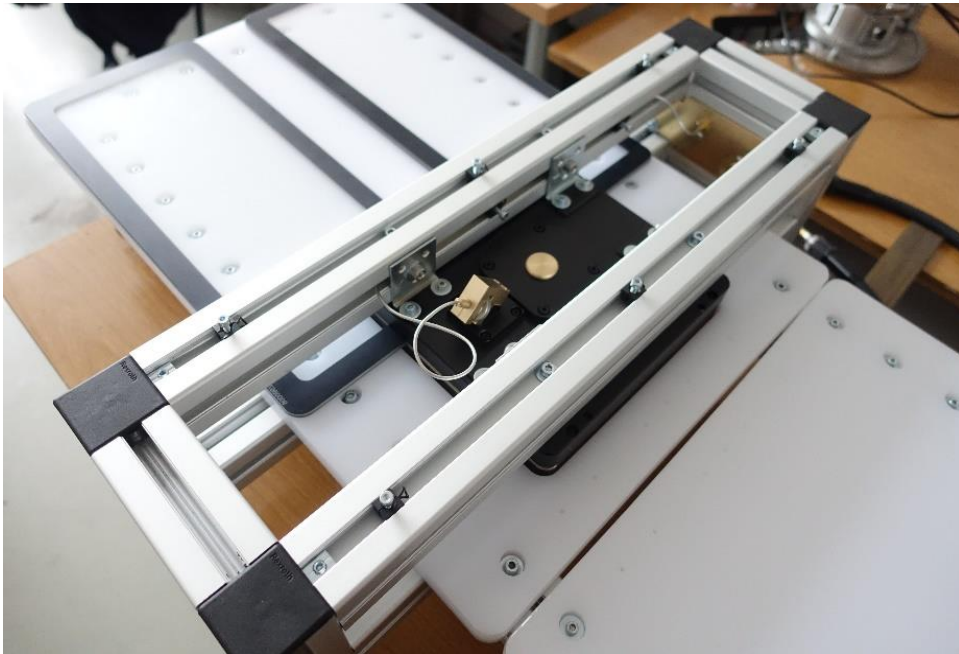
liquids & powders  
*can also heat*

# Surface scanning with SPDR

## Obviating 1st out of 3 limitations:

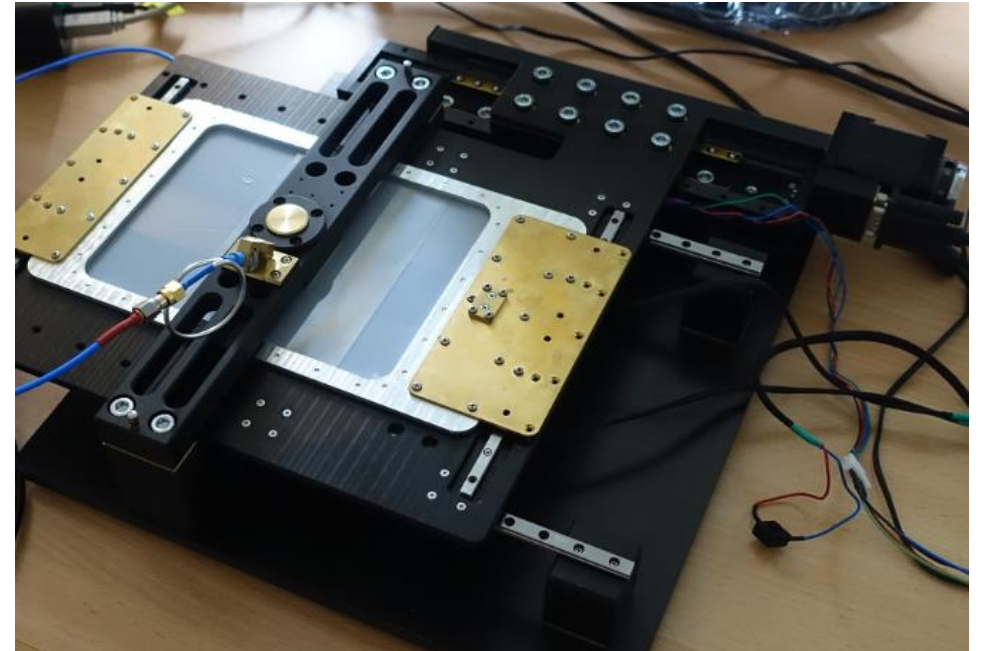
- SUT thickness - slot size 0.6..6 mm
- SUT lateral min size ("absolute" EM constraint) - 14..120 mm
- spatial resolution 14..120 mm
- SUT lateral **max size** (mechanical construction) – 40..150 mm

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



Cambridge, 29-31 May 2019

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



NEMO 2019



# Automatic surface scanning with SPDR



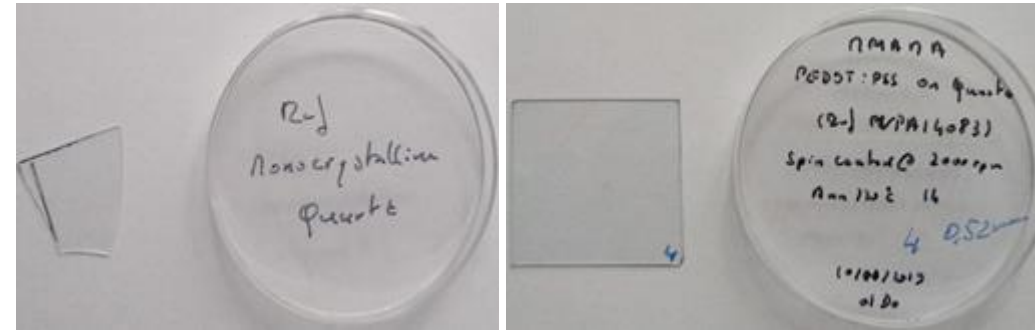
working with QWED Q-Meter

Cambridge, 29-31 May 2019

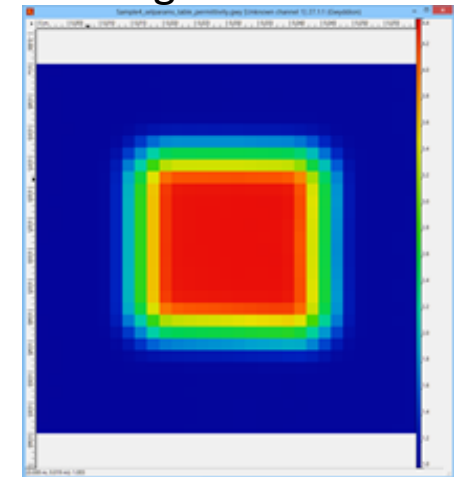
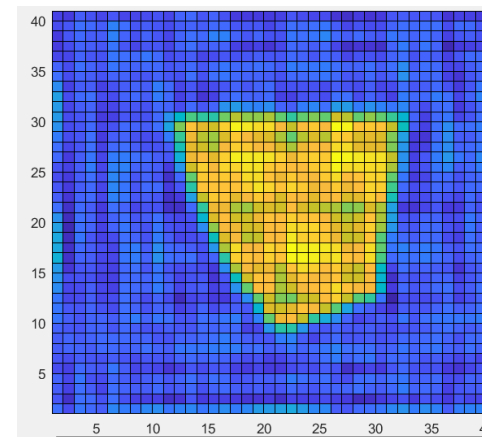


working with FieldFox  
(Keysight hand-held VNA)

NEMO 2019



samples from MateriaNova  
quartz substrate & deposited organic material

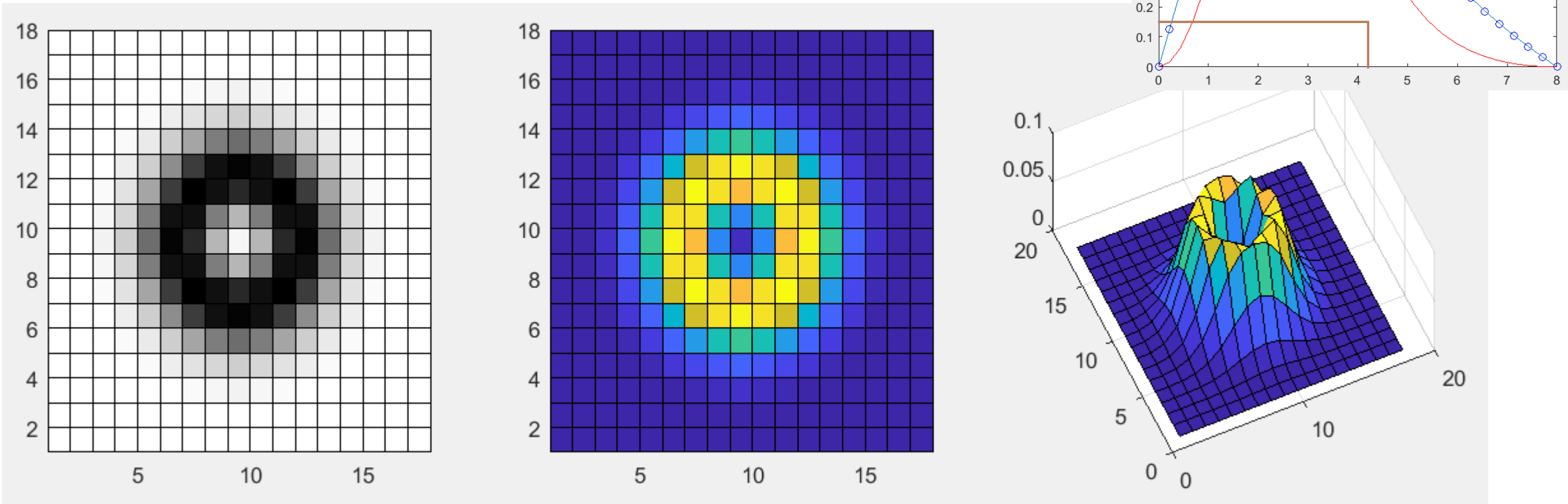


scanning step 1mm  
but resolution ~16mm !  
→ seek modelling-based  
resolution enhancement

# 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:



# 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  $a$  ( $a = 1\text{mm}$  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  $\Delta W_i, i=(n-1)*M+m, i=1, \dots, M*N$ , 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 :

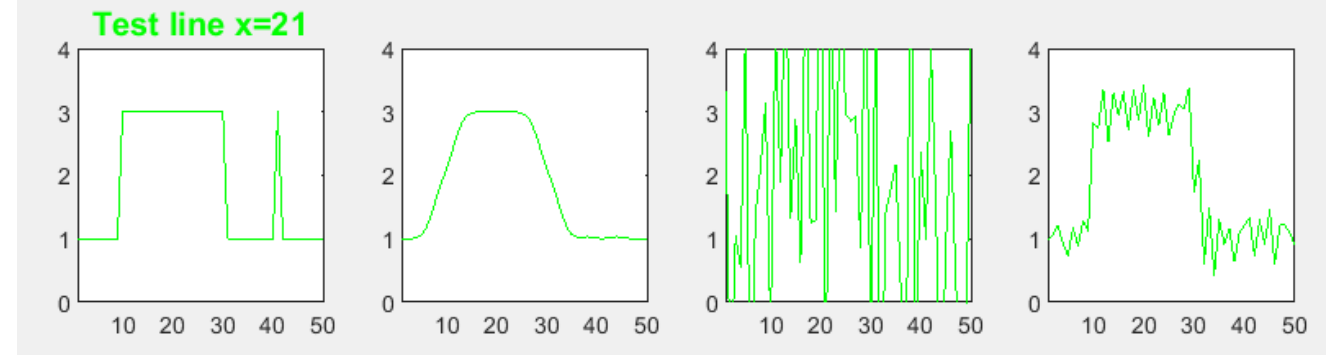
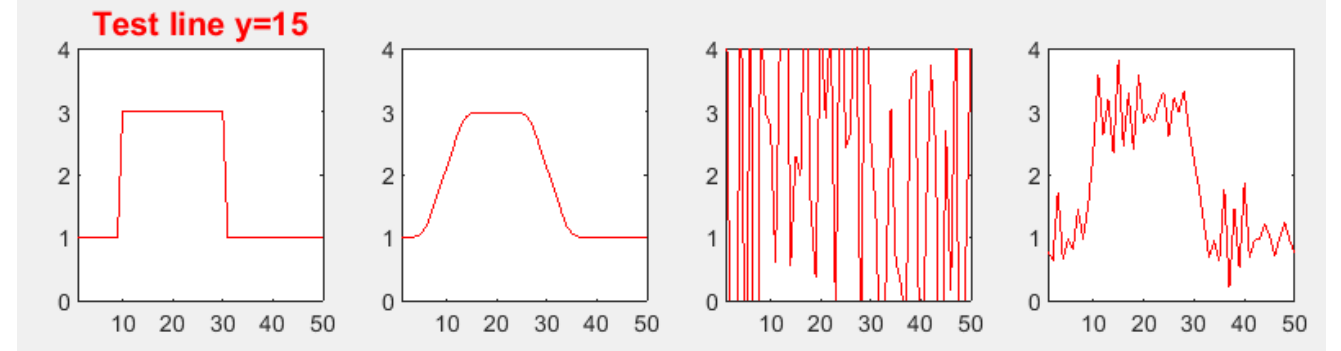
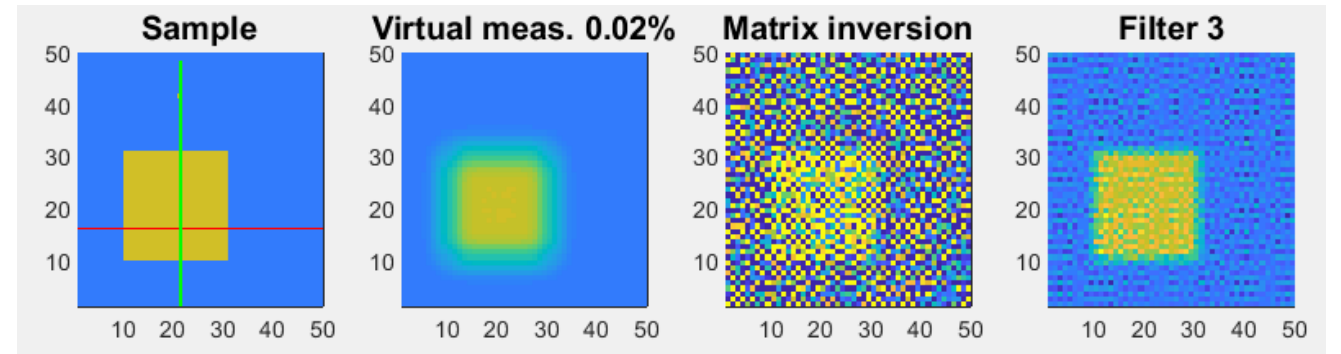
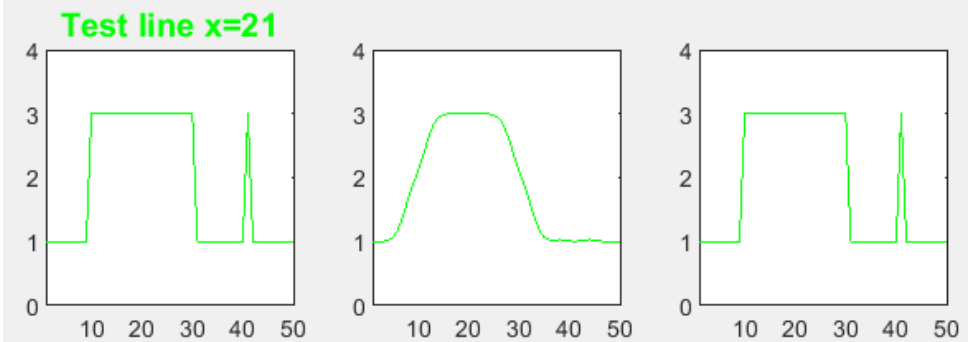
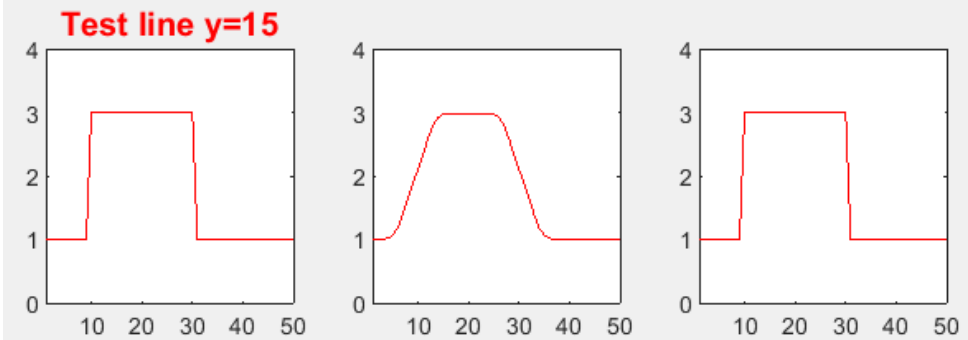
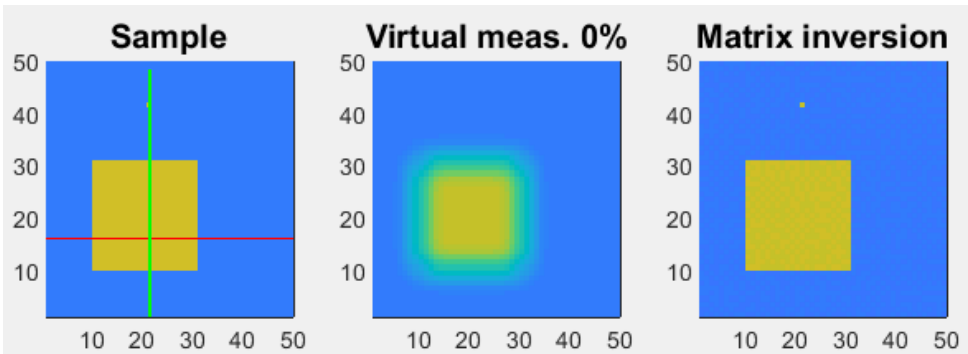
- $|E_T(k, l)|^2$  for  $s = r + k + Ml$  for  $k = -K \dots +K$  and  $l = -L \dots +L$
- 0 for  $s$  not obeying the above condition.

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

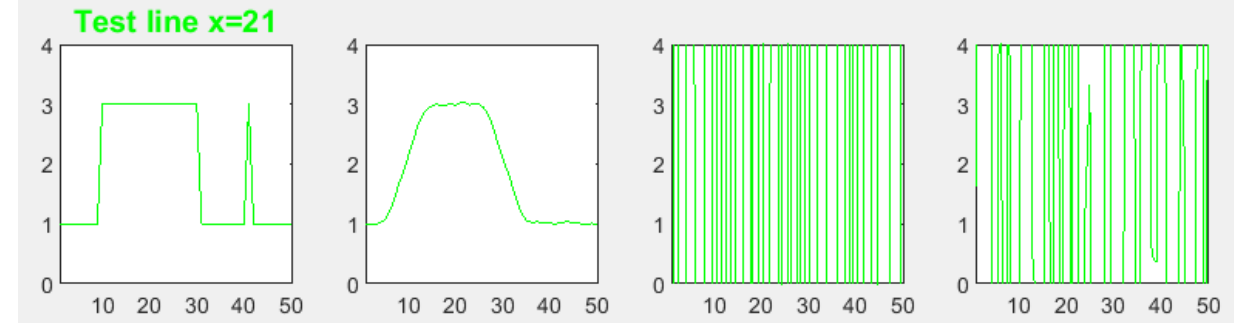
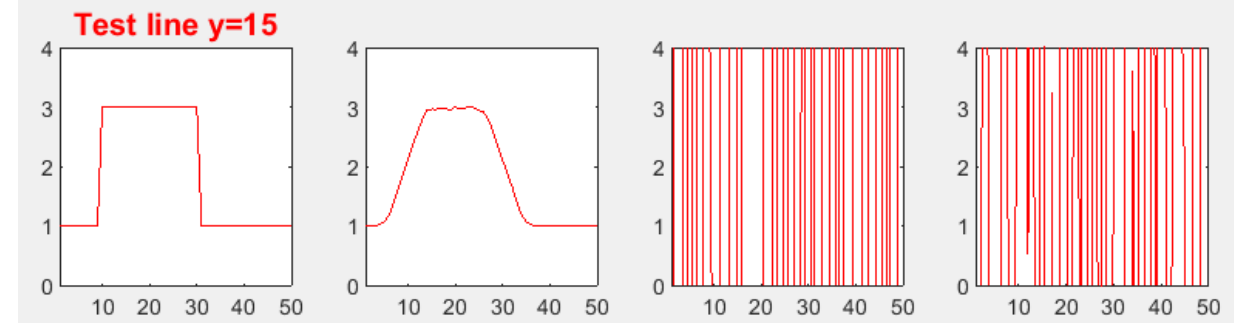
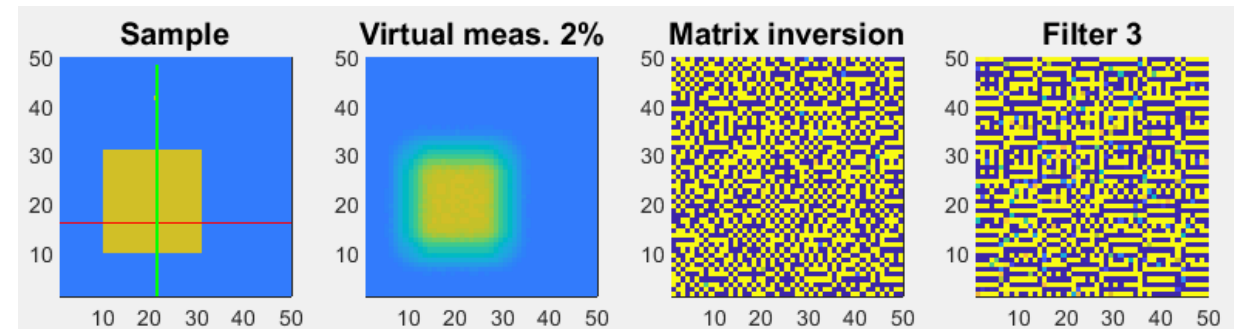
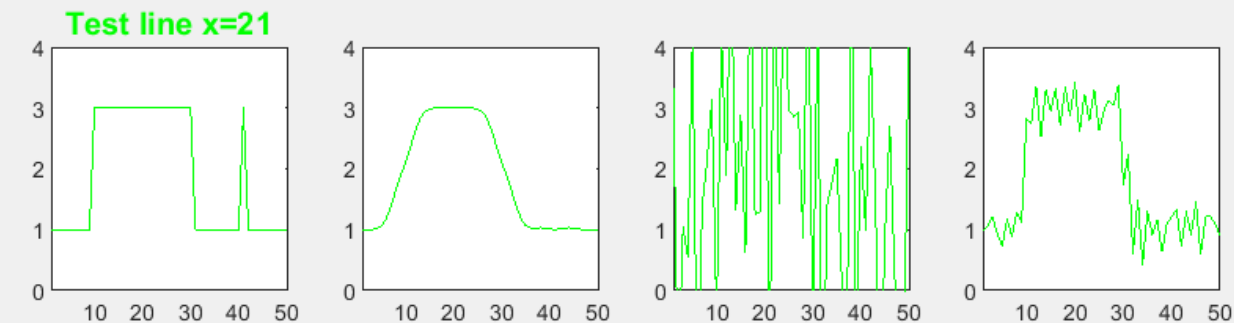
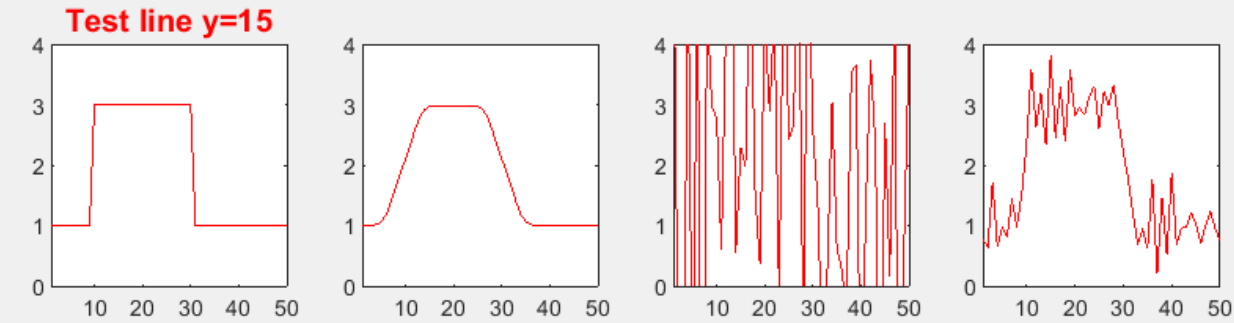
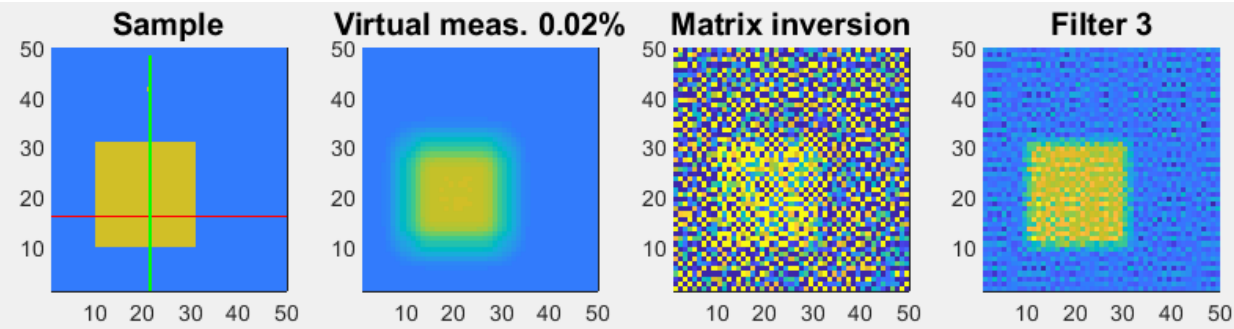
Matrix  $T$  is large,  $M*N \times M*N$ , but sparse and has a banded structure.

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

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

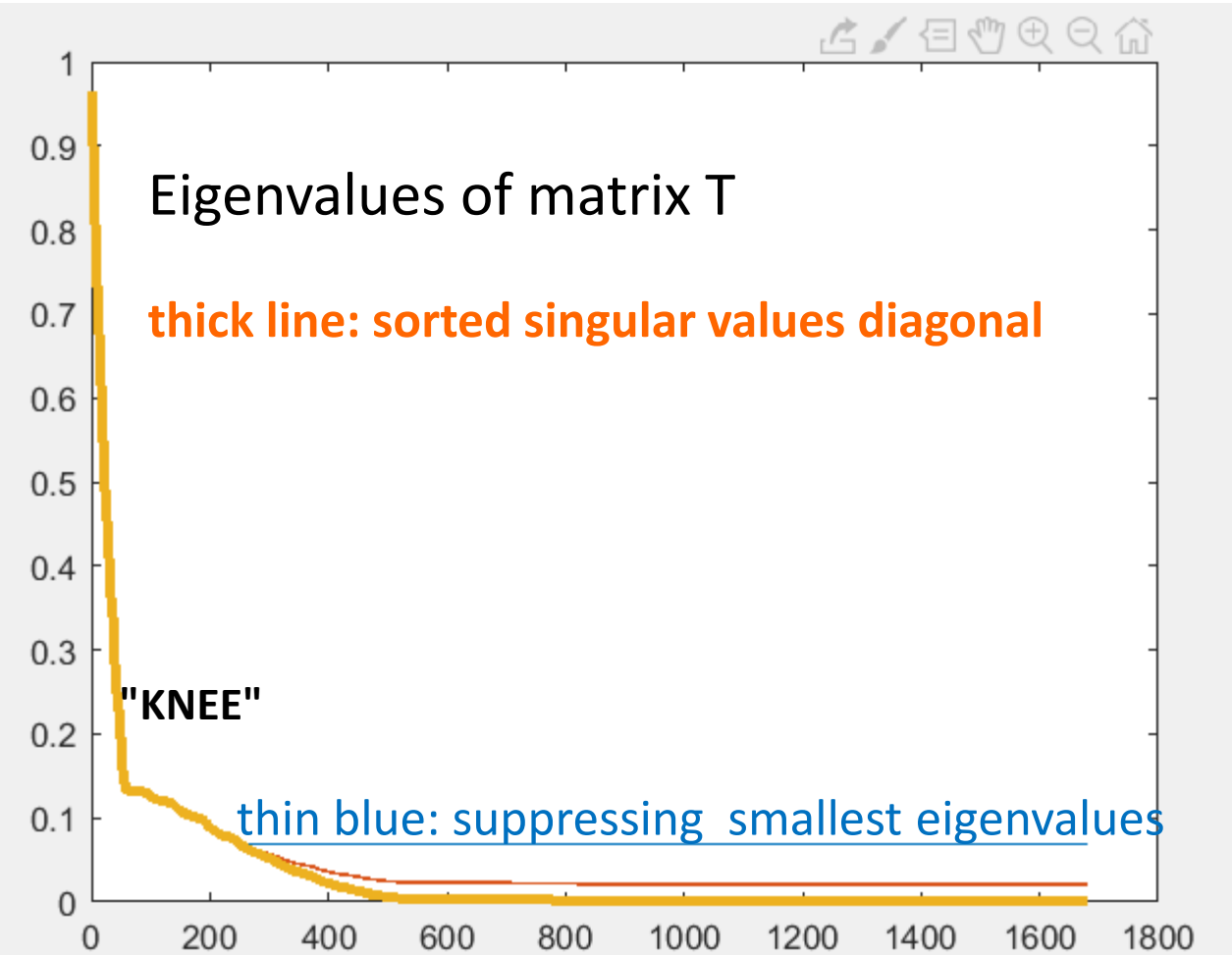


# MATLAB experiments with virtual scans: matrix inversion with increased noised

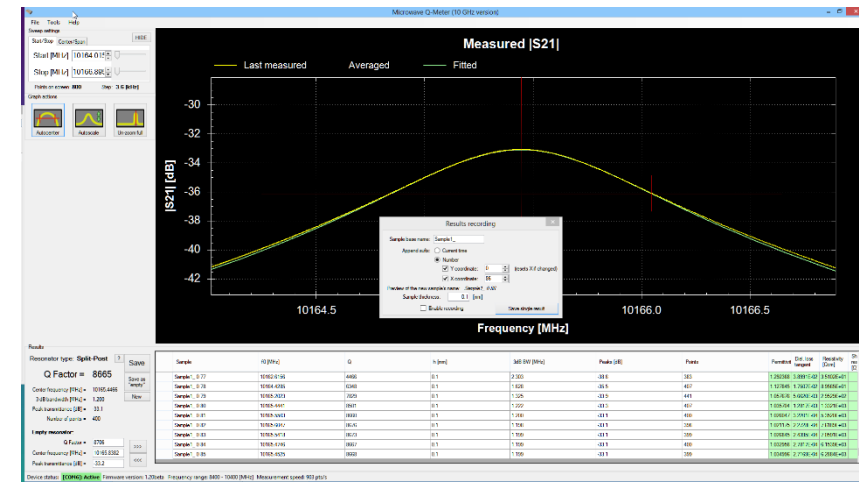




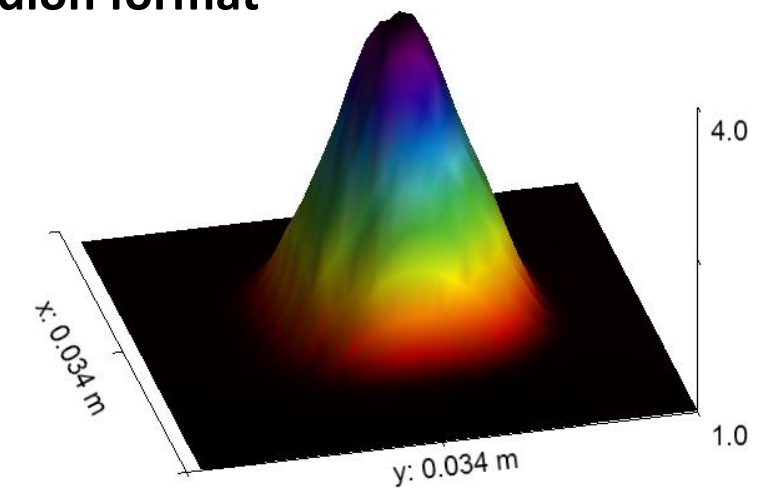
# Singular Value Decomposition



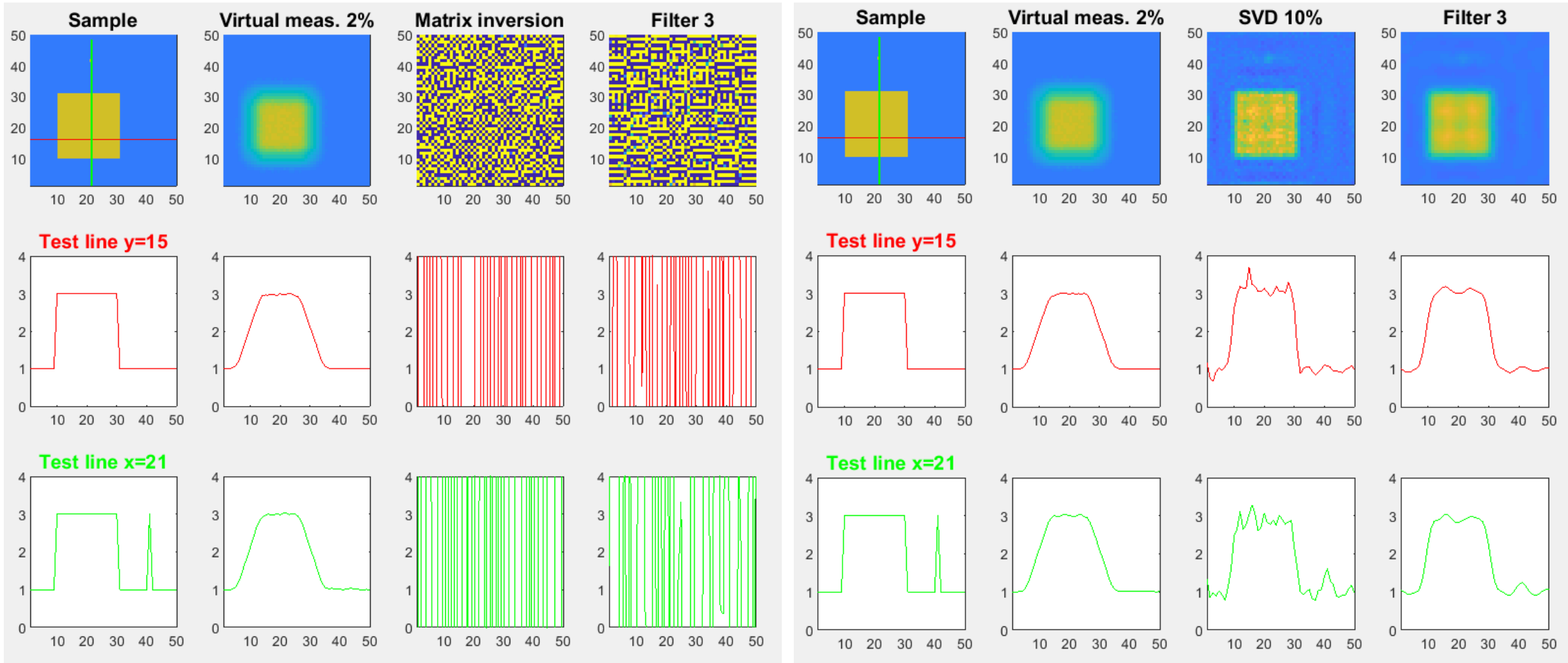
thin red: searching for balance between stability & accuracy



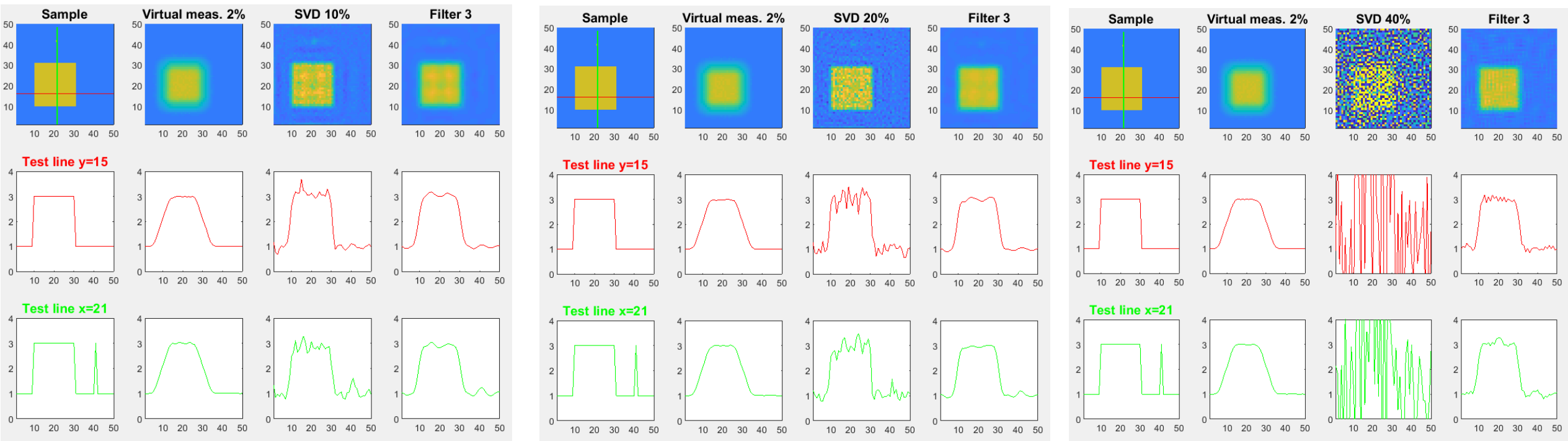
scan area 41x41mm  
 => matrix 1681x1681 (step 1mm)  
 SUT laminate Rogers R4003 h=20mils (0.508 mm)  
 SUT size 15x15 mm  
 scan saved in Gwyddion format



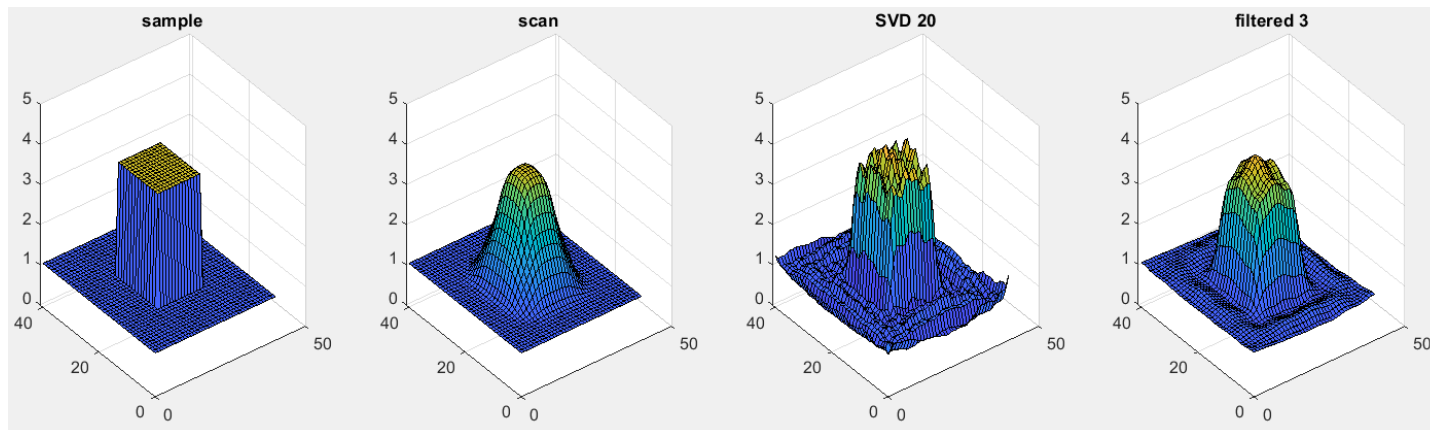
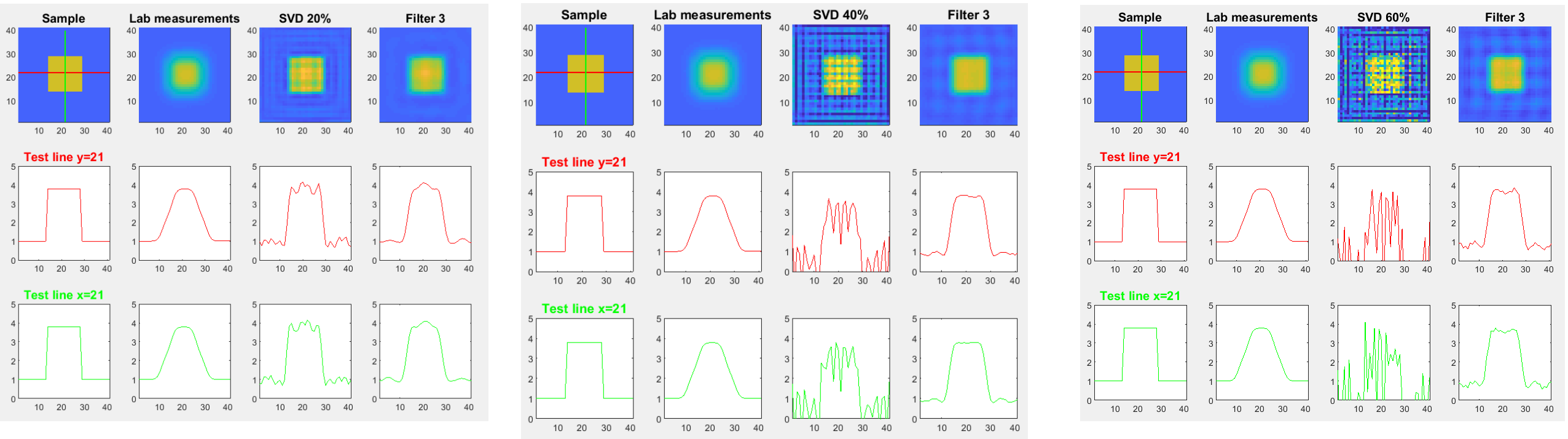
# MATLAB experiments with virtual scans: matrix inversion versus SVD approach



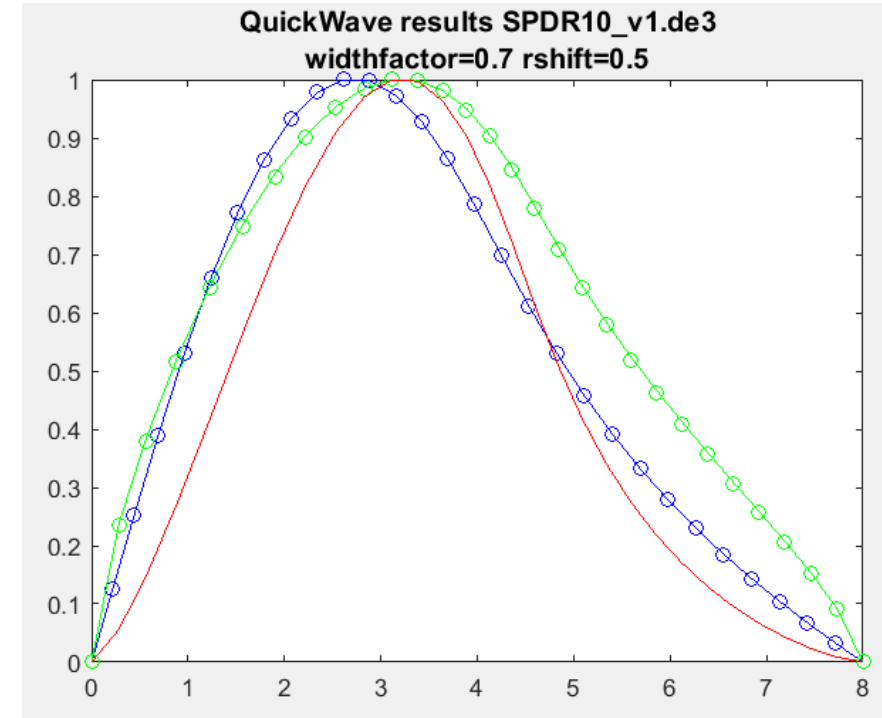
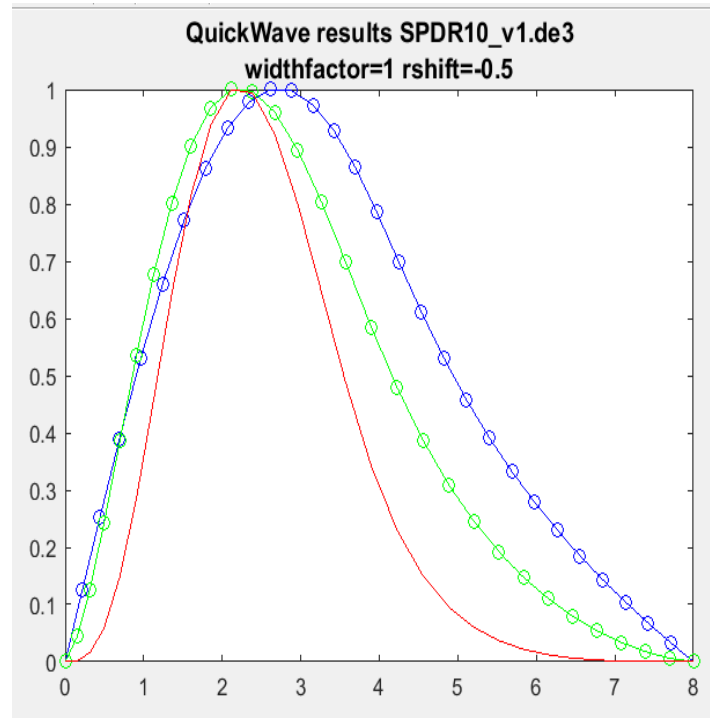
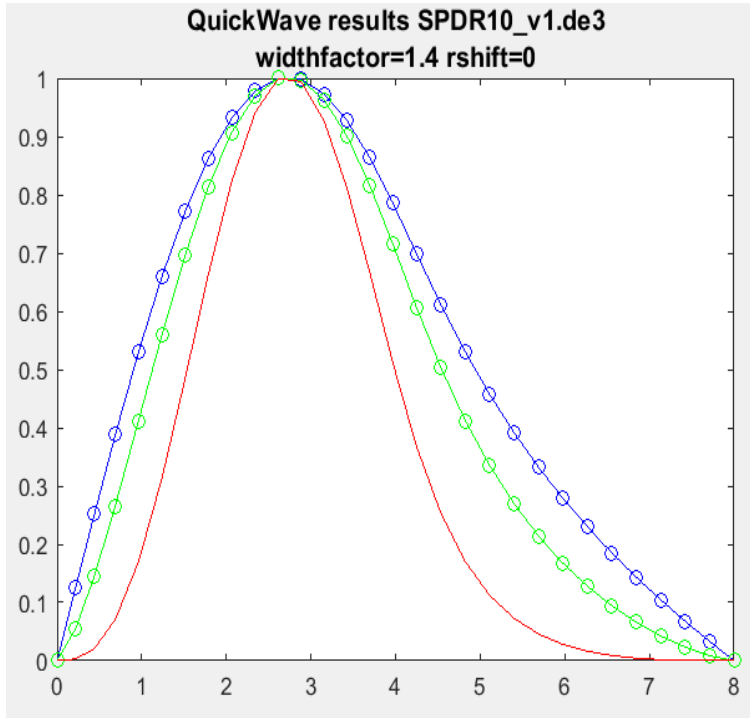
# MATLAB experiments with virtual scans with error: experimenting with SVD parameters



# MATLAB experiments with laboratory scans: experimenting with SVD parameters



# MATLAB experiments with laboratory scans: experimenting with templates



**Note: each SPDR requires calibration -> field pattern after manufacturing differs from the theoretical design.**

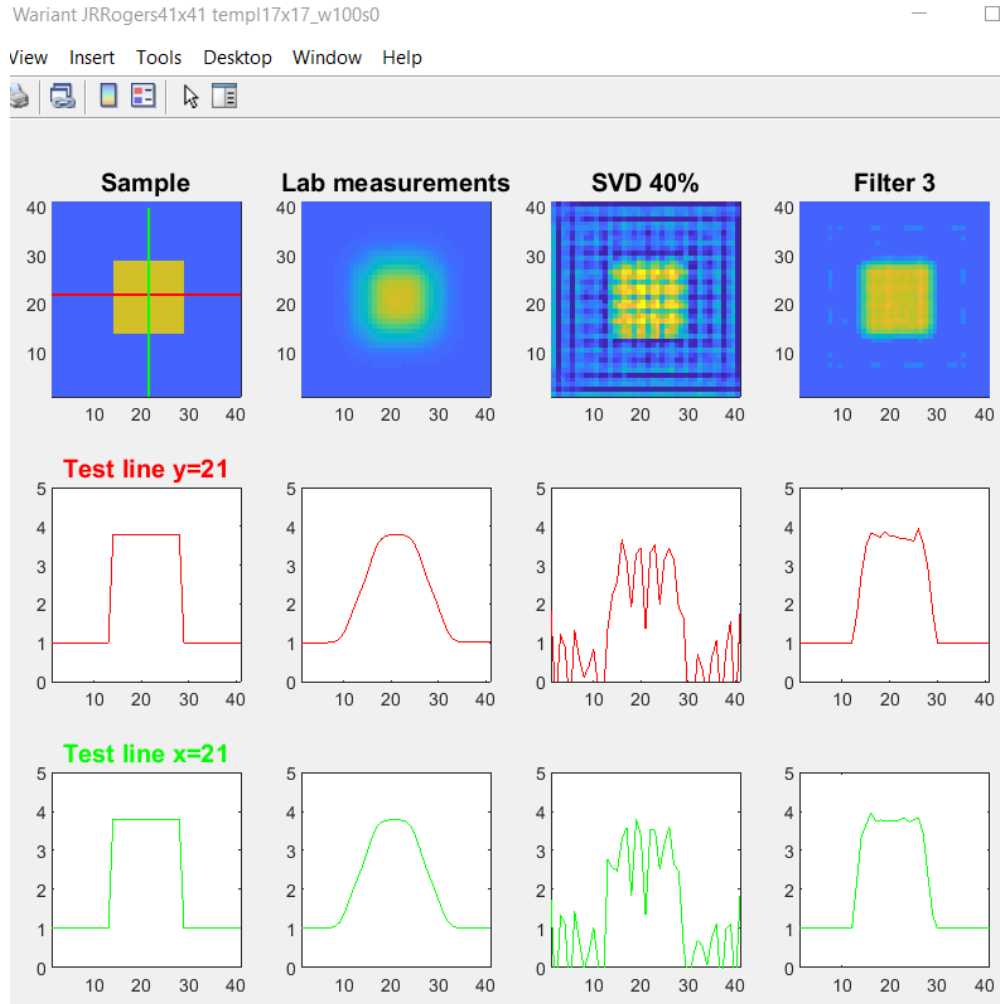
blue – QuickWave simulation of E-field for theoretical SPDR design, interpolated in MATLAB

green – modified ("narrowing" or shift)

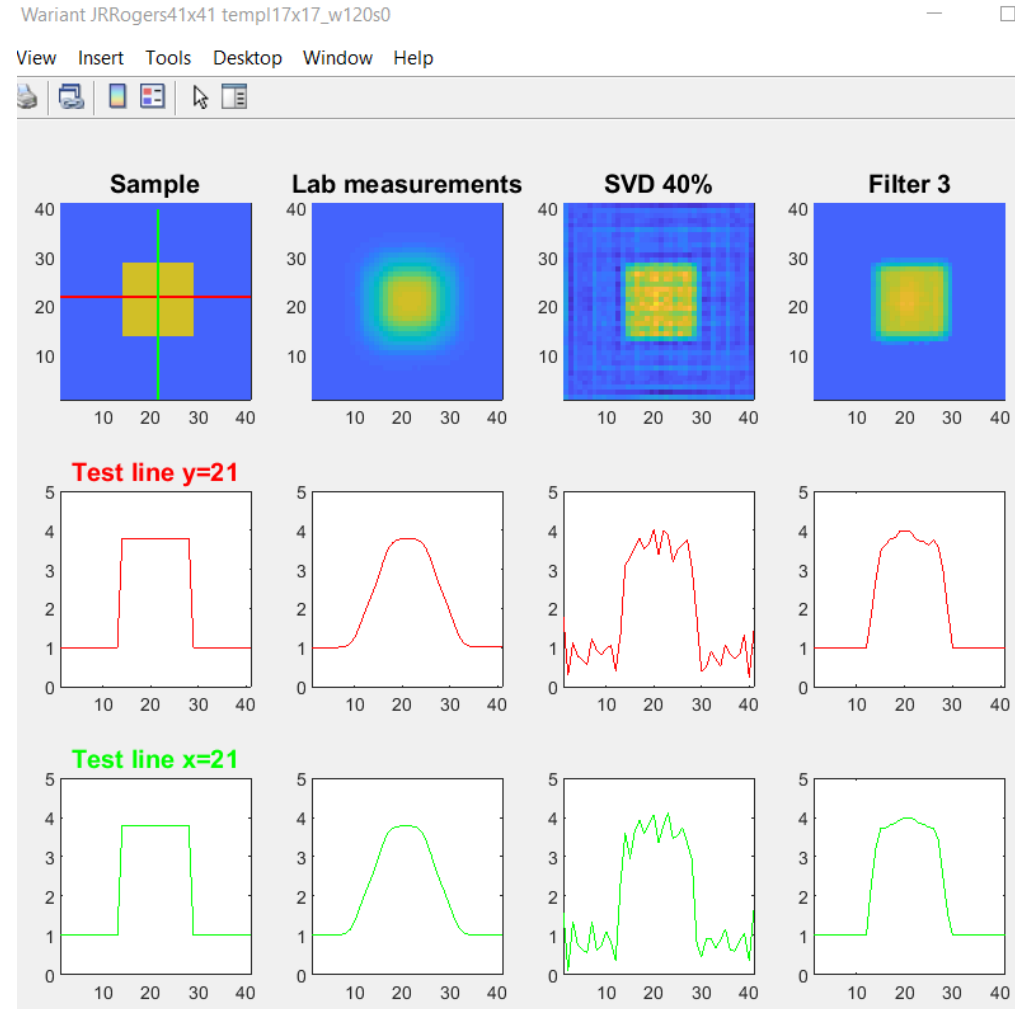
red – modified squared



# MATLAB experiments with laboratory scans: experimenting with templates (1)

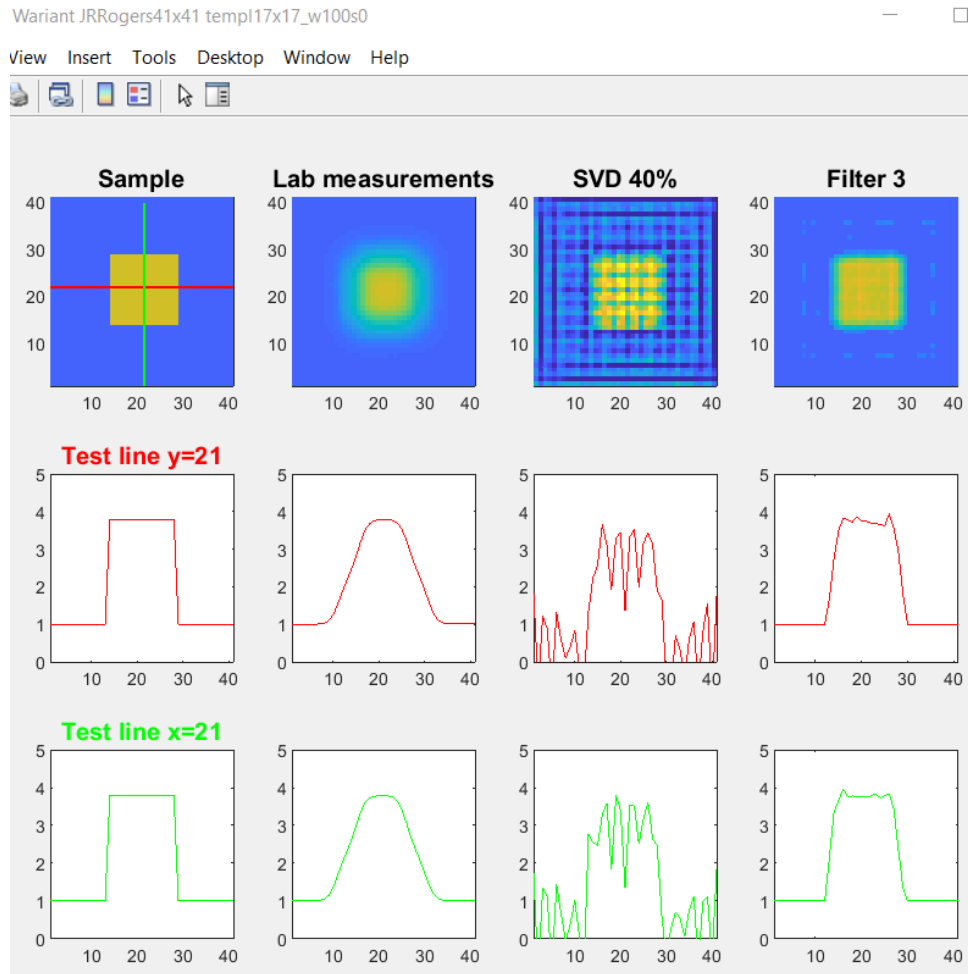


**original template**

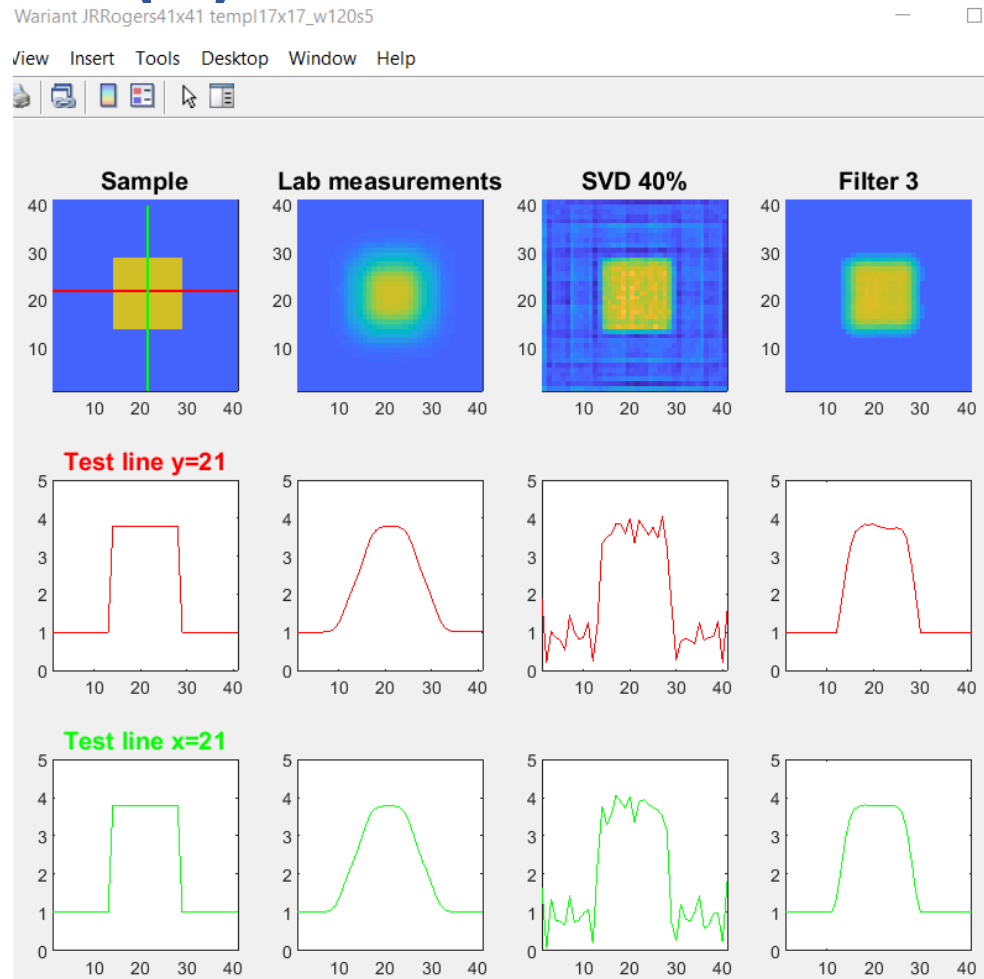


**stronger energy concentration in ring:  
"narrower" template  $E^{1.2}$**

# MATLAB experiments with laboratory scans: experimenting with templates (2)

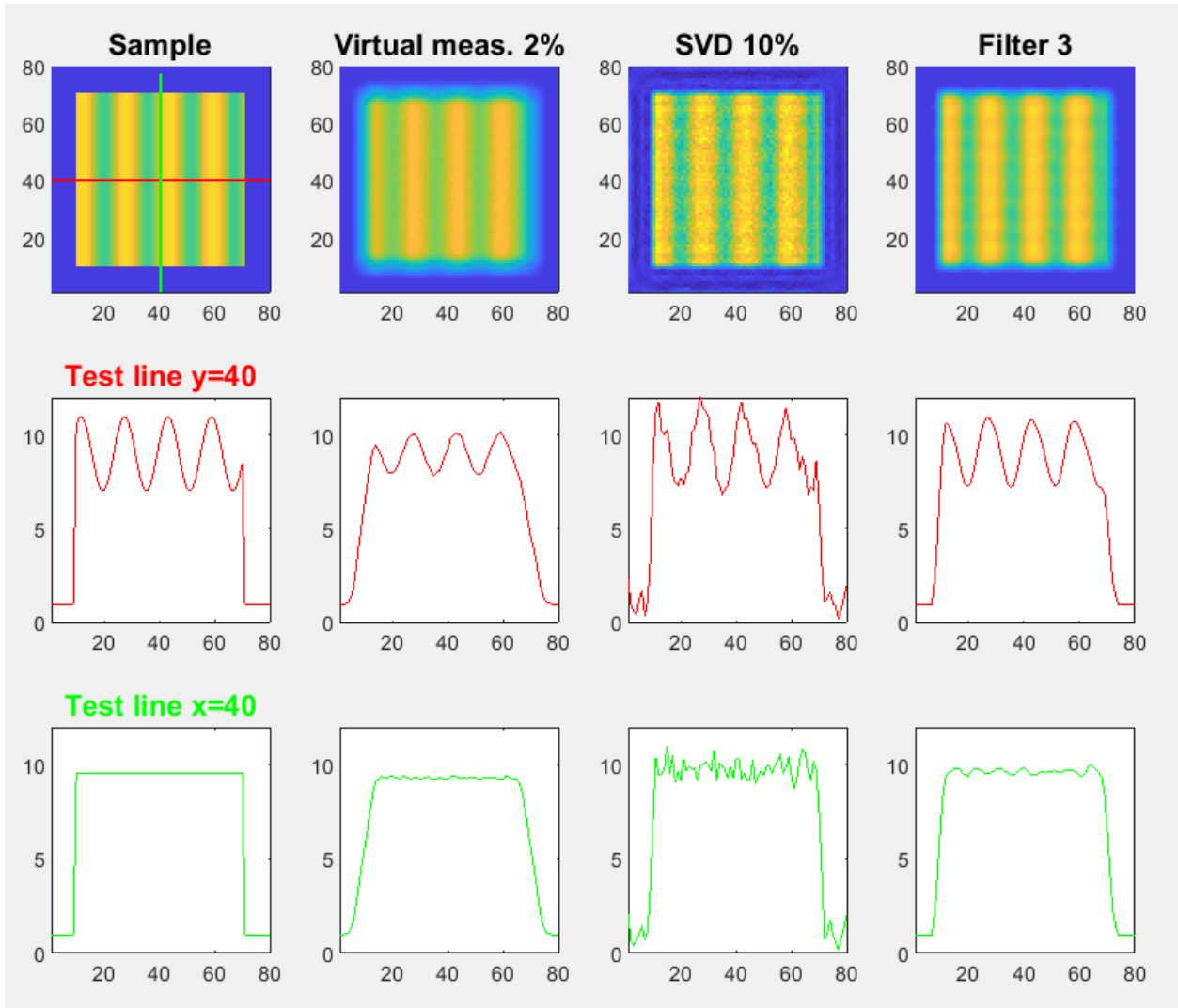


original template



"narrower" template  
stronger energy concentration in ring: template E<sup>1.2</sup>  
further shifted by 0.05 mm

# MATLAB experiments with virtual scan: continuous permittivity distribution



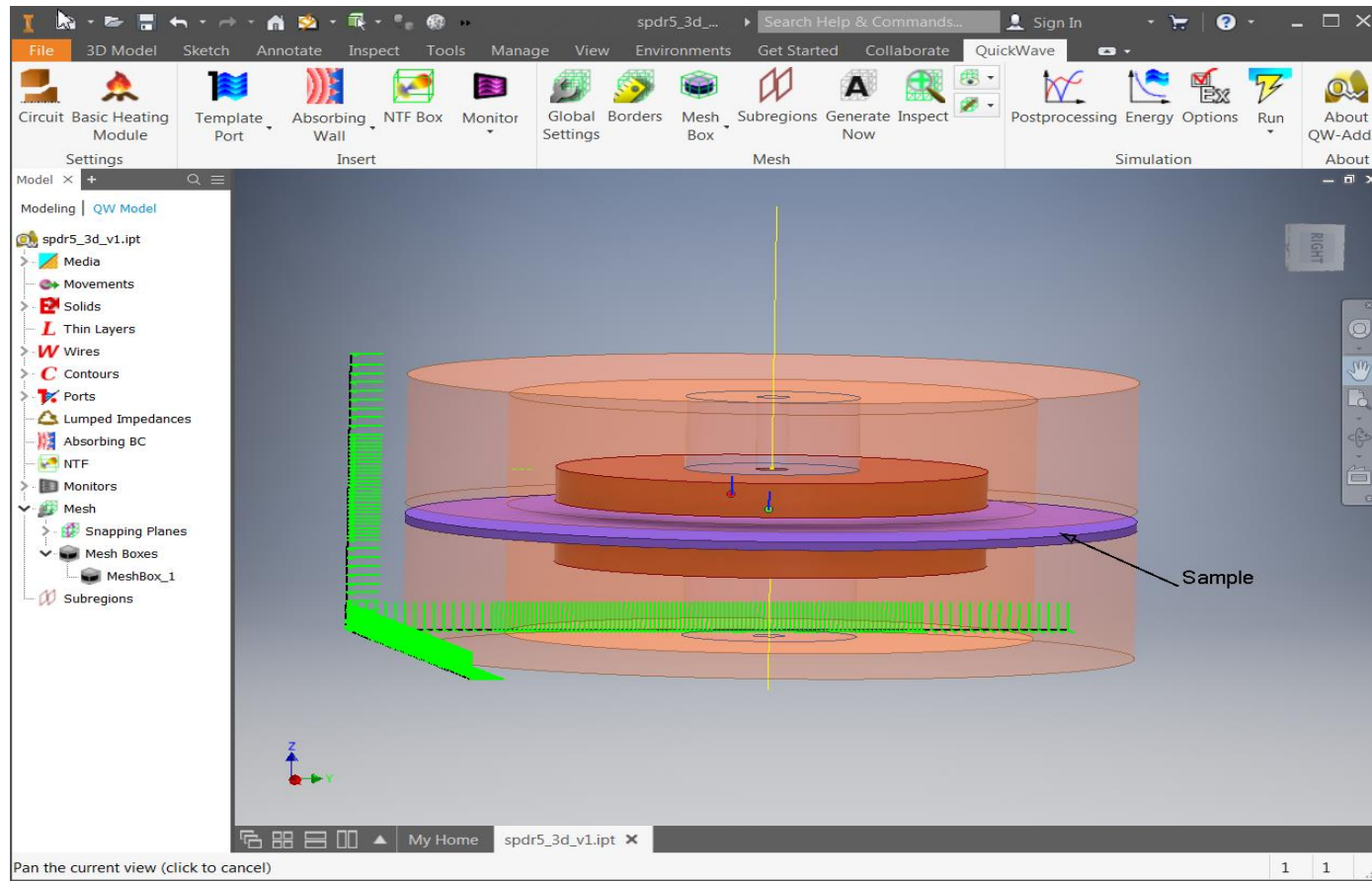
**Virtual permittivity pattern,  
corresponding to radial resistivity pattern  
measured on wafer.**

**Different resolution criteria in two directions:  
horizontal – continuous pattern  
vertical – sharp edges;  
both enhanced with SVD method.**

# Modelling validation of SPDR method assumptions

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

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



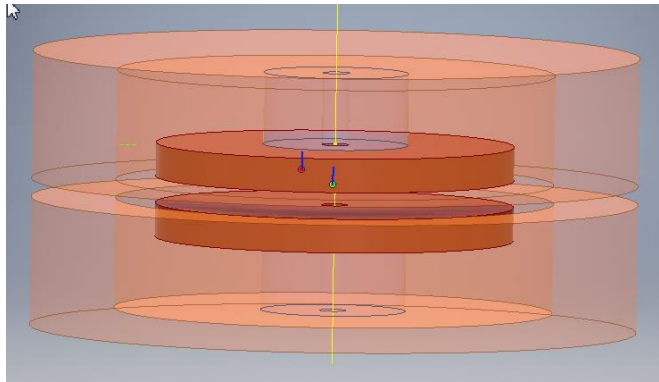
10 GHz SPDR model in **QW-AddIn** for Autodesk® Inventor® Software

# Modeling validation of SPDR method assumptions

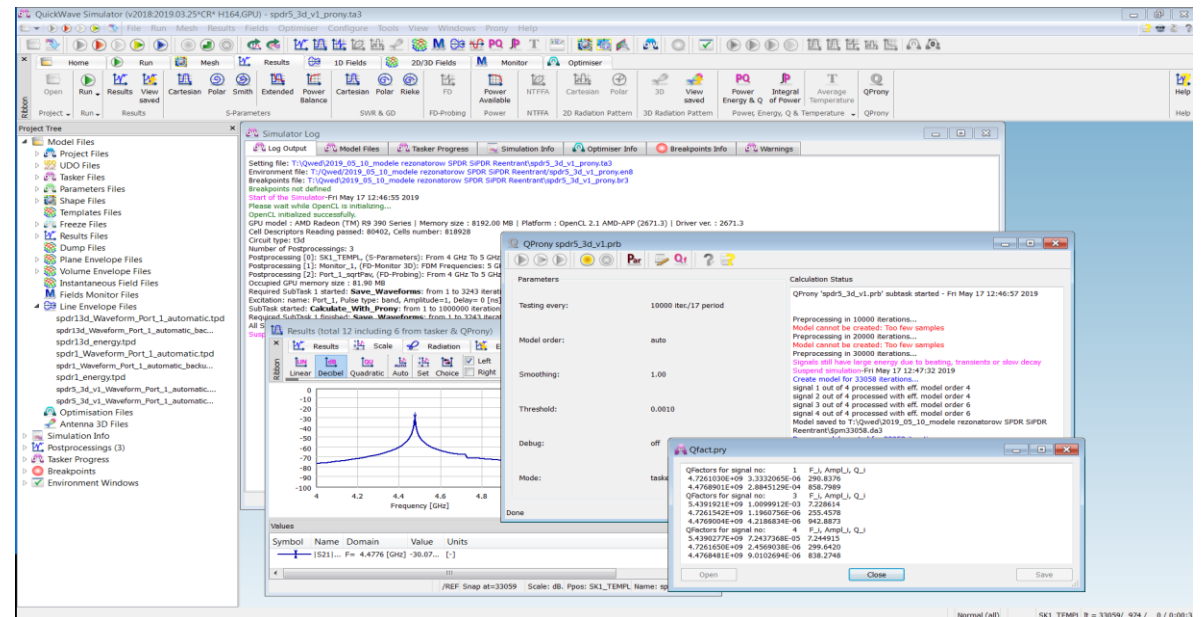
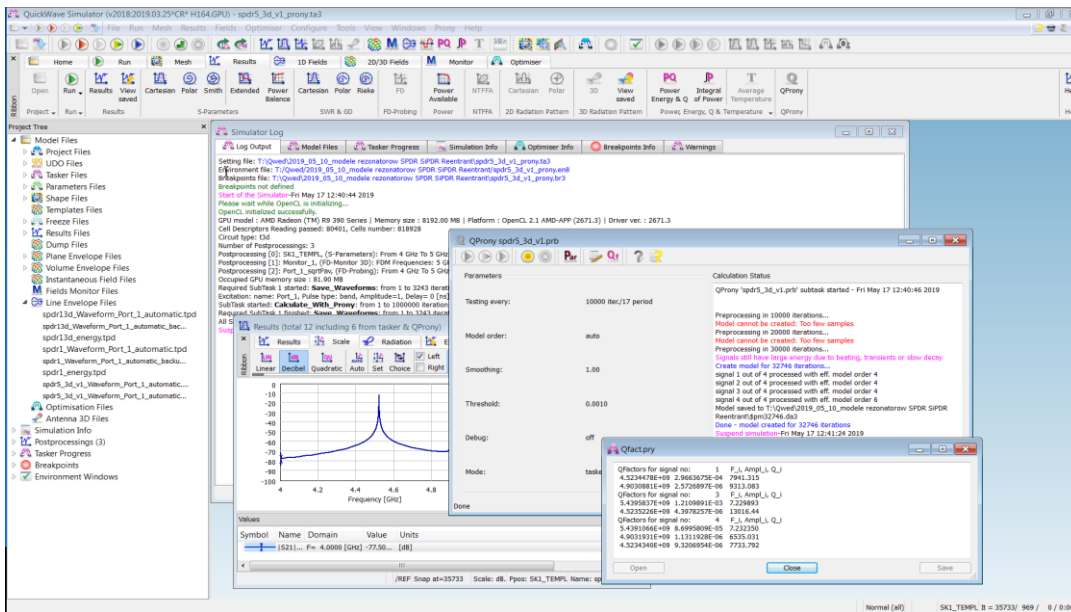
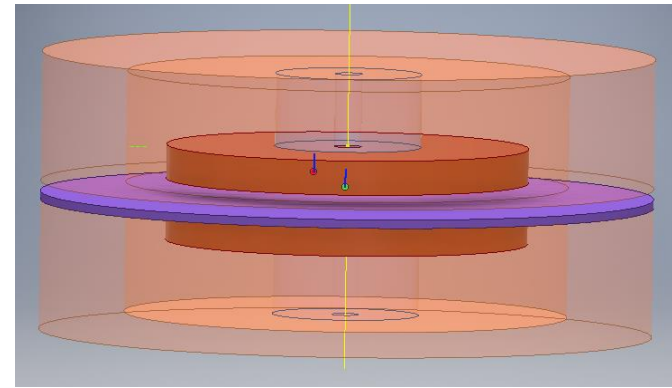
How much is the E-field pattern influenced by SUT?

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

empty



with SUT

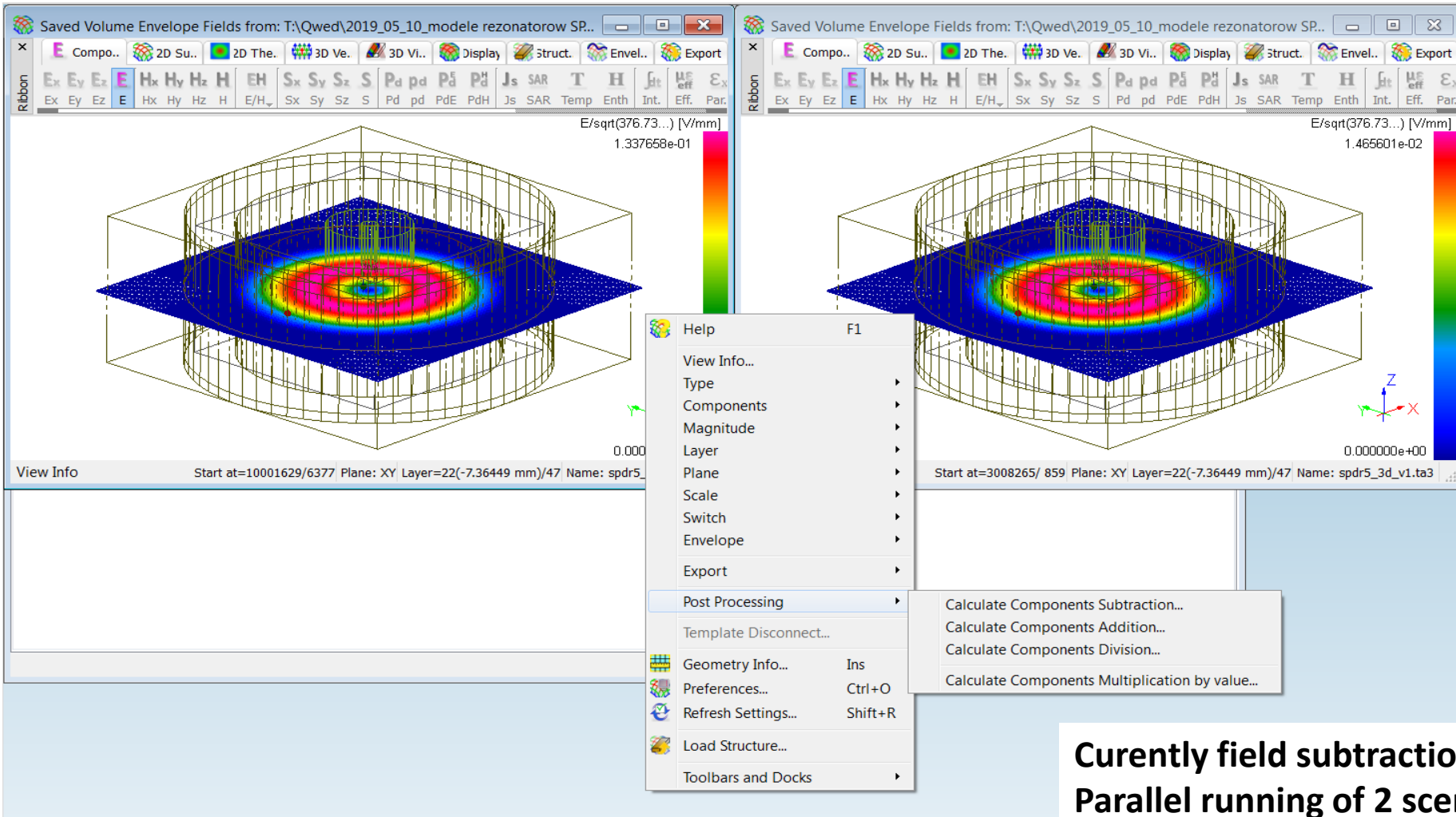




# Modelling validation of SPDR method assumptions

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

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

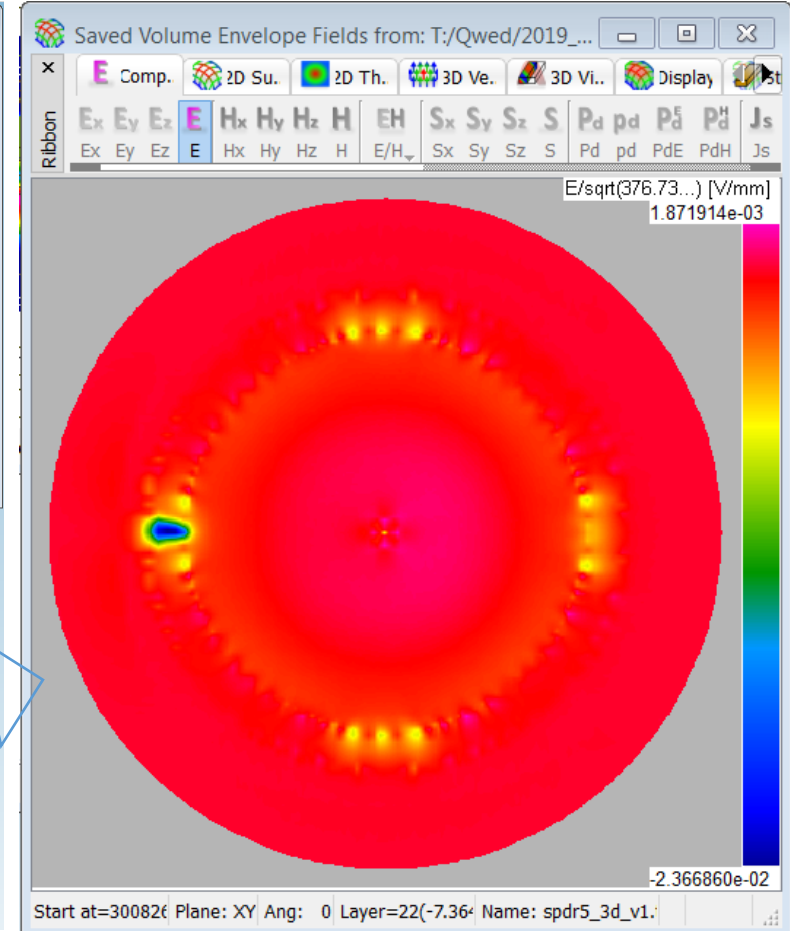
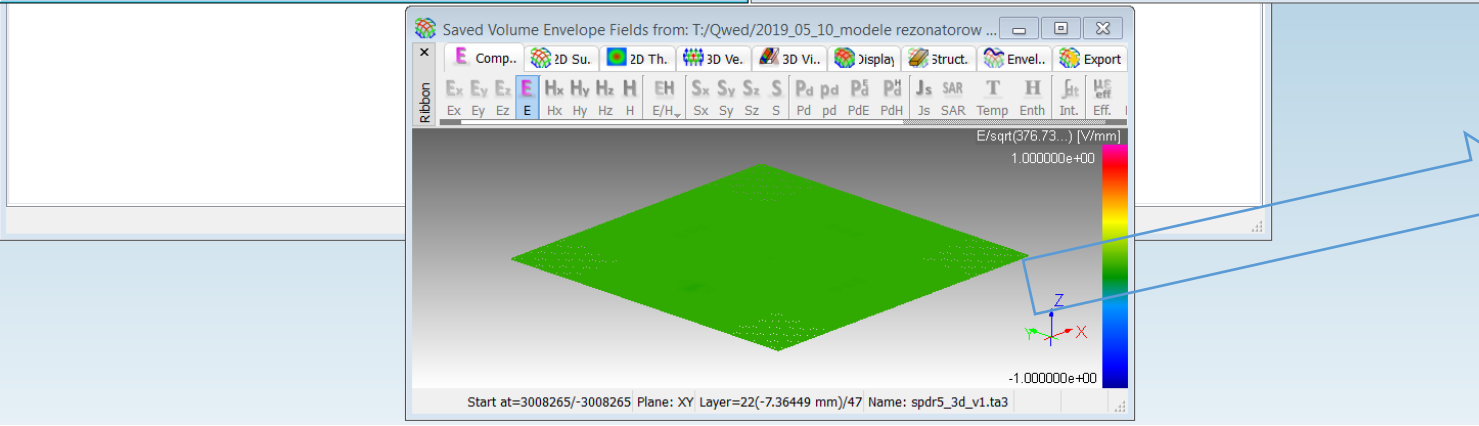
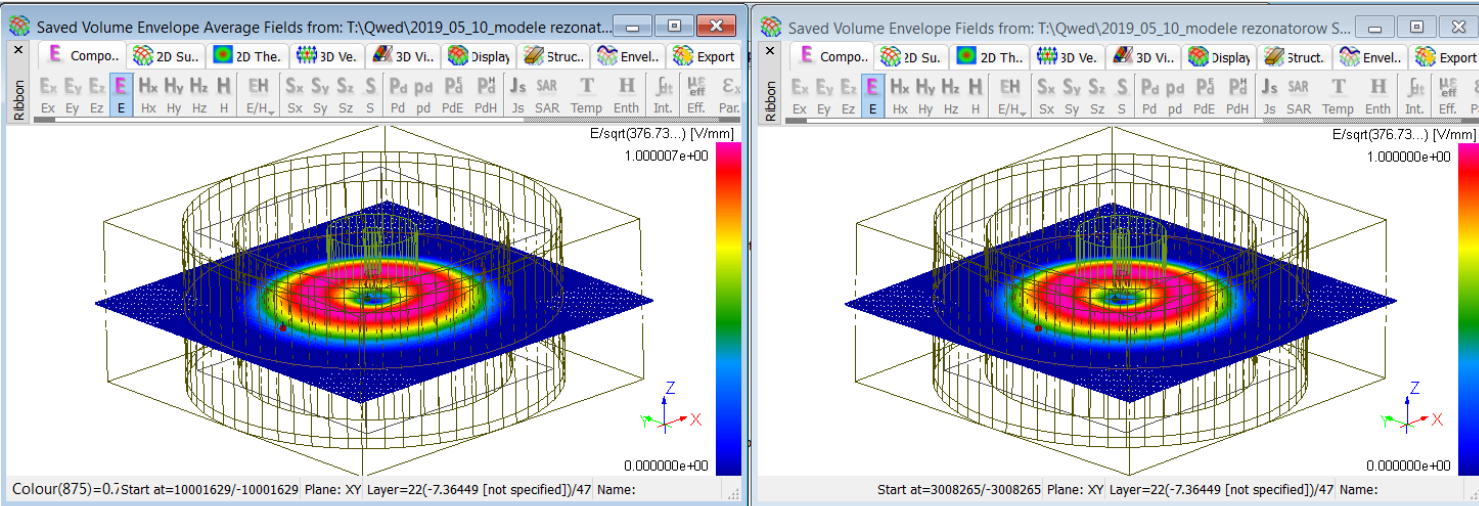


**Currently field subtraction performed on saved fields.  
Parallel running of 2 scenarios under development.**

# Modelling validation of SPDR method assumptions

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

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

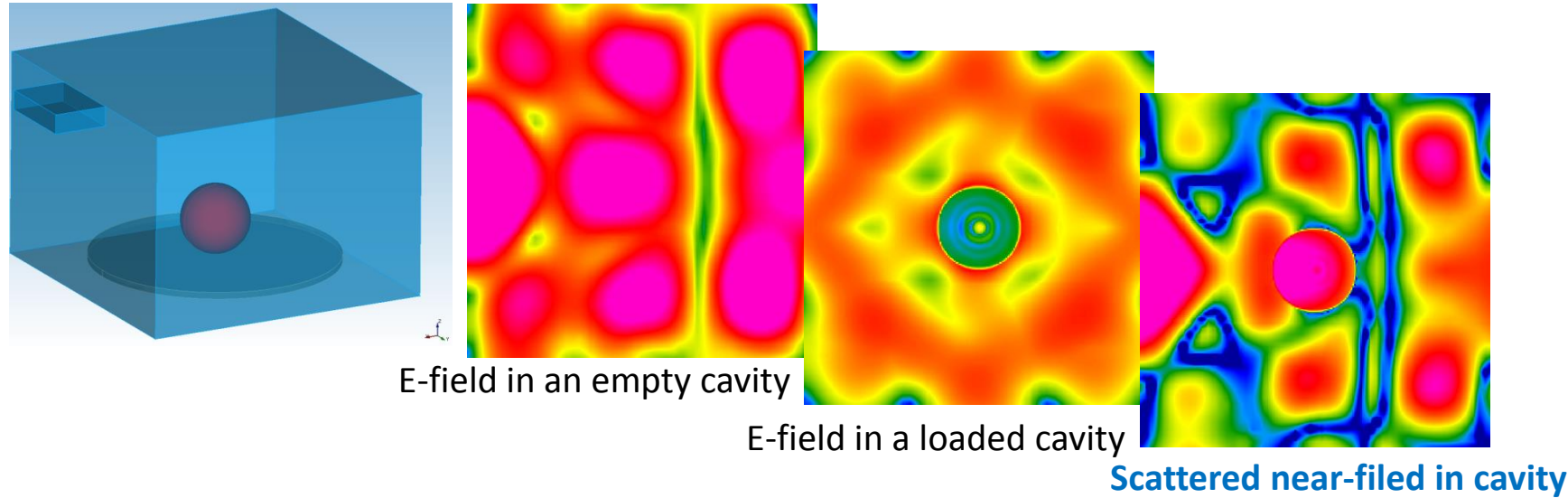


~ 0.2%

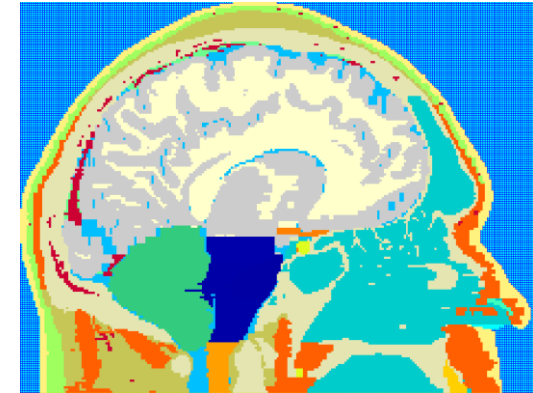
- 0.2%

# Advanced near-field imaging functionality

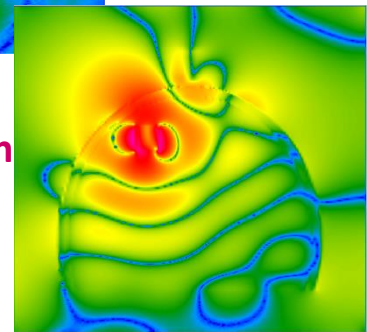
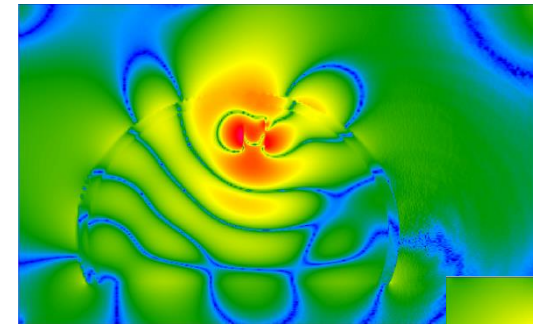
Separation of incident and diffracted fields (*option implemented per request of P.O.Risman, Malardalen Univesity*)



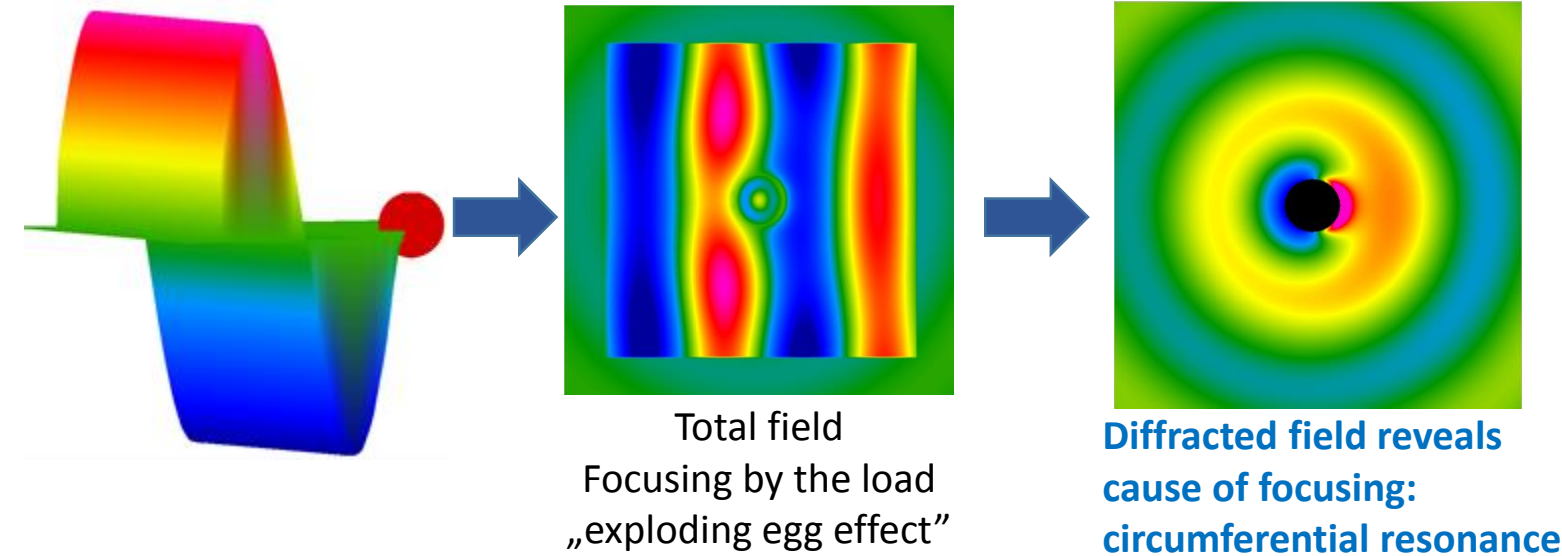
## Detection of inhomogenities in tissues



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



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



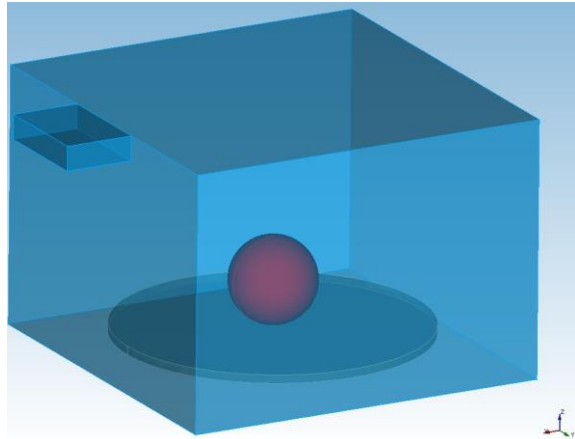


# Accurate modelling of coupled electromagnetic-thermal problems

## Application to

Simple microwave heating benchmarks  
& microwave heating phenomena studies\*

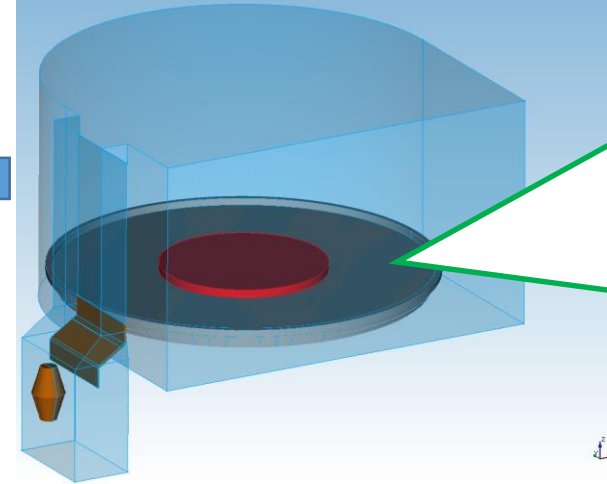
Design & analysis of real-life microwave oven cavities, incl.  
complicated cavity shapes and advanced feeding system\*



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

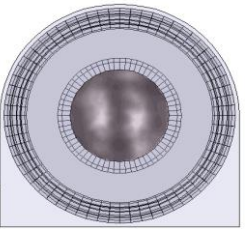
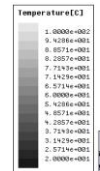
Freezing to file  
the state of the  
simulation

De-freezing on  
arbitrary computer  
& at convenient  
time

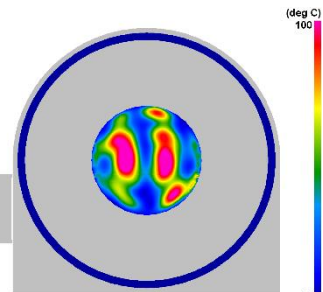


Courtesy of Whirlpool Inc. – Whirlpool MAX oven

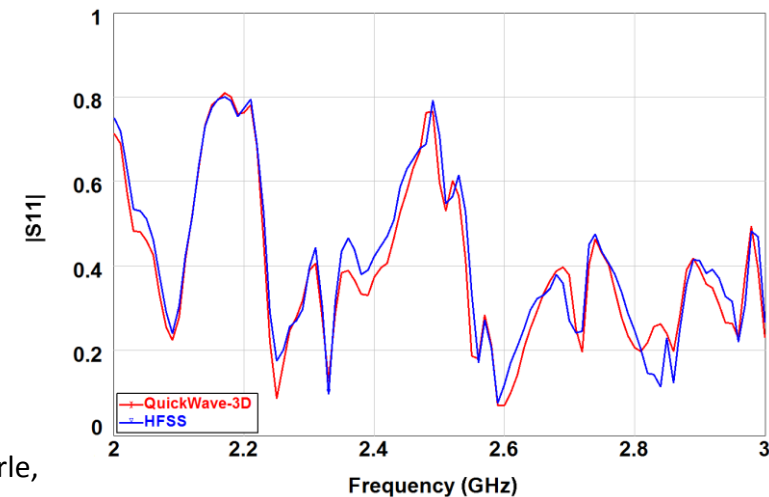
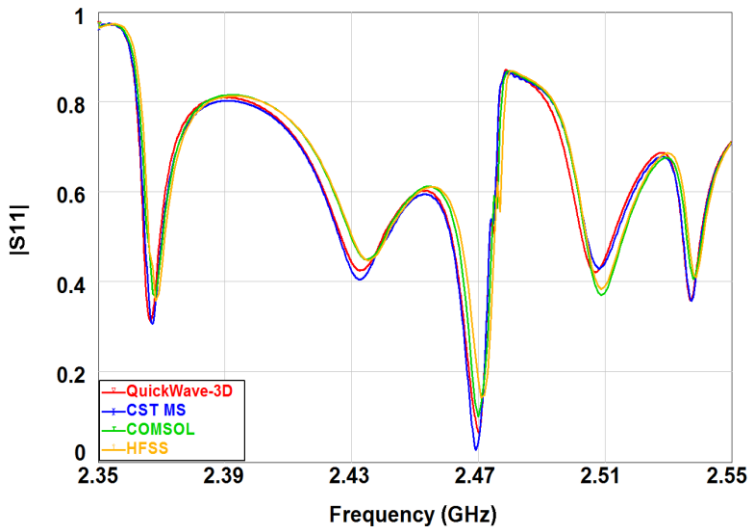
HFSS v11



QuickWave 3D & BHM

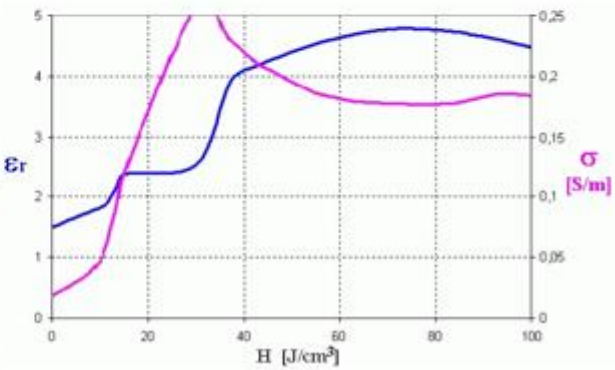
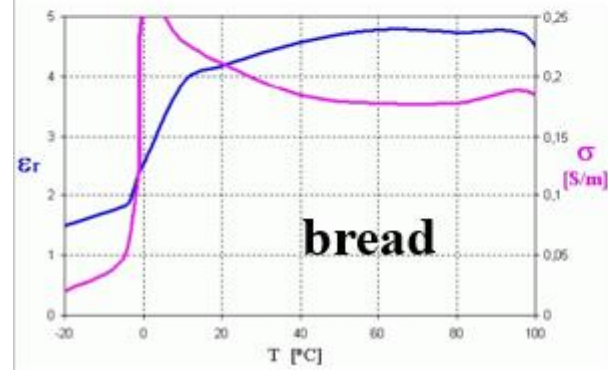
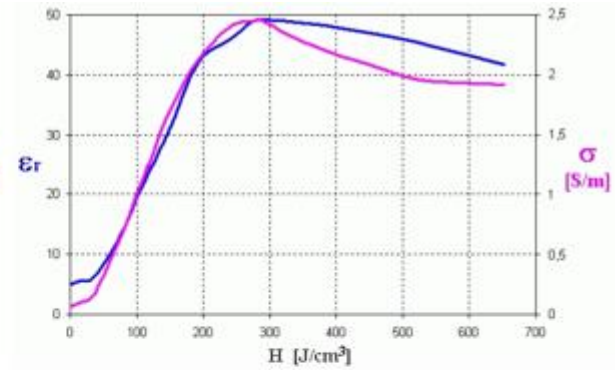
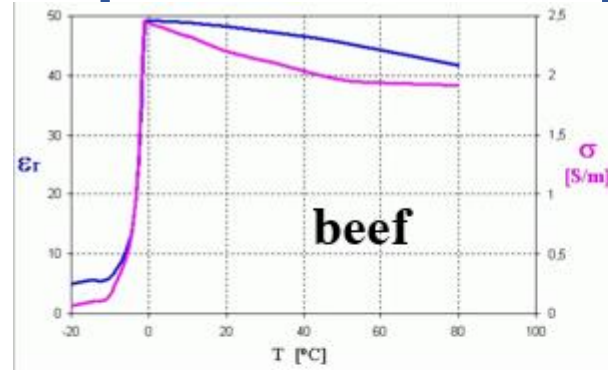
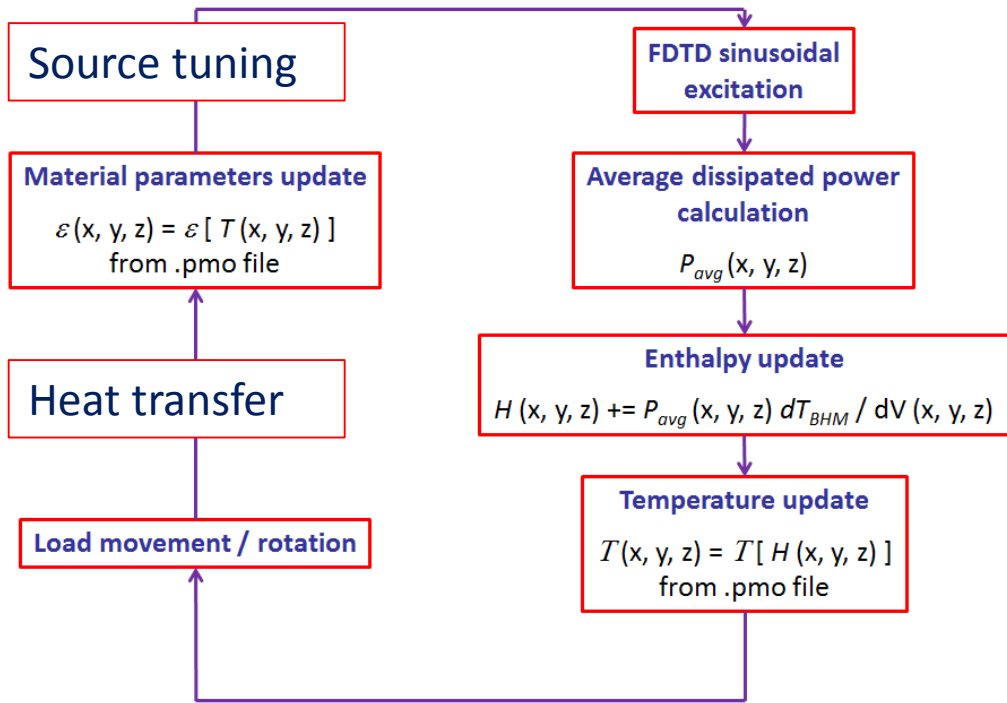


With QuickWave EM  
computation as fast as  
**1 min 18s** on a **low-cost  
video card** – supporting  
**all graphic cards with  
OpenCL**

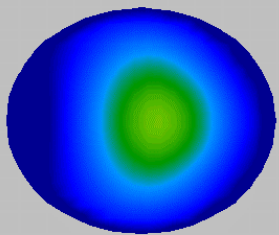


\* Considered by M.Celuch, P.Kopyt & M. Olszewska-Placha in eds. M. Lorence, P. S. Pesheck, U. Erle, *Development of packaging and products for use in microwave ovens*, 2nd Ed. Elsevier in print.

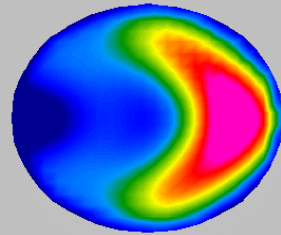
# Multiphysics modelling: temperature-dependent materials



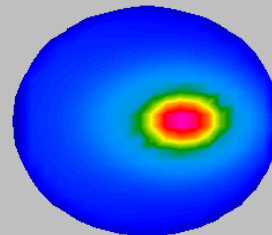
-20 deg.



+20 deg.



7 thermal steps



varying 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*

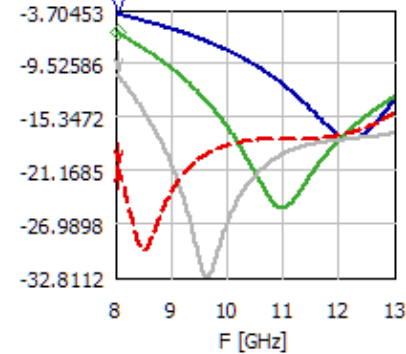
**Collect Data** of S11 and dissipated power density in potato heated in MW oven, as text files and GUI

Type	Name	Status
Results	S-Parameters Results	Window
	S-Parameters Cumulative Results	Cumulative Window
Radiation Pattern	Radiation Pattern Results	Window
	3D Radiation Pattern Results	Window
Fields	Fields	Window
	Fields	Window
Monitor	Monitor	Window

Open Windows at first run - suspend simulation at: last iteration

Add | Configure... | Delete | Clear

- S-Parameters Results
- S-Parameters Cumulative Results
- 2D Radiation Pattern Results
- 3D Radiation Pattern Results
- Fields
- Monitor



Symbol	Name	Domain
—v	[S11] (GS=1)	F = 8.0000 [GHz]
—◇	[S11] (GS=2)	F = 8.0000 [GHz]
—v	[S11] (GS=3)	F = 8.0000 [GHz]
- - -+	[S11] (GS=4)	F = 8.0000 [GHz]

$\epsilon_r$  changing from 10 to 80

Grid Search Steps: 8, Iterations per Simulation=40000  
 Number of Objectives: 1  
 \*Objective 1: Collect, WindowsNb=3  
 Window 1: Fields, "Fields"  
 Window 2: Fields, "Fields"  
 Window 3: Fields, "Fields"

Grid Search=1: Variable(s): eps\_potato=10-  
 Grid Search=2: Variable(s): eps\_potato=20  
 Grid Search=3: Variable(s): eps\_potato=30  
 Grid Search=4: Variable(s): eps\_potato=40  
 Grid Search=5: Variable(s): eps\_potato=50  
 Grid Search=6: Variable(s): eps\_potato=60  
 Grid Search=7: Variable(s): eps\_potato=70  
 Grid Search=8: Variable(s): eps\_potato=80+

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

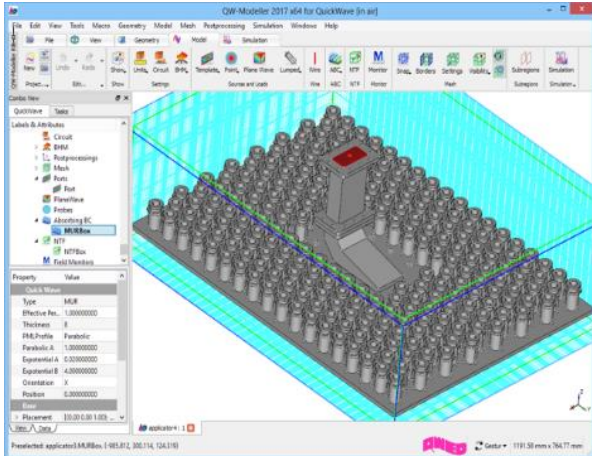


# Unusual QuickWave applications

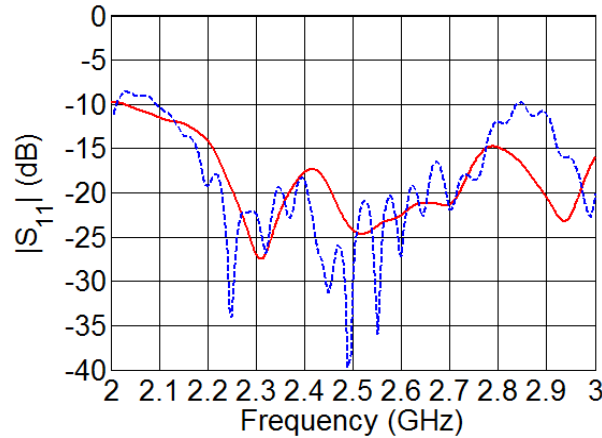
High power applicator for  $\mu\text{W}$  treatment of bituminous surfaces aiming at road repair

**Challenges**

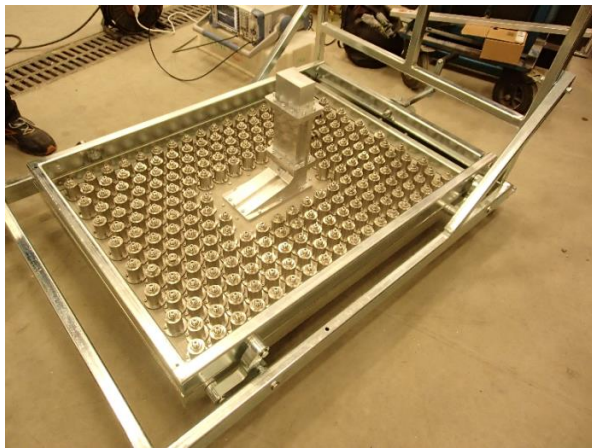
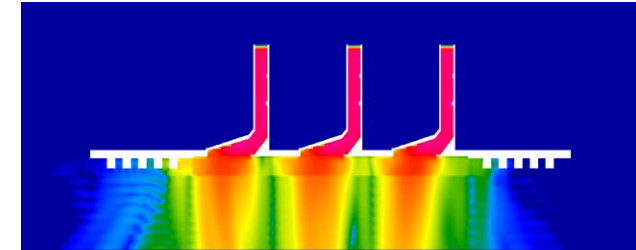
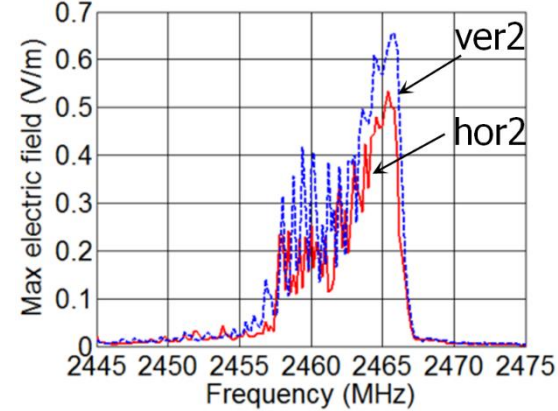
- High dissipation of  $\mu\text{W}$  power in road surface
- Safety issues – prevention of EM energy leakage



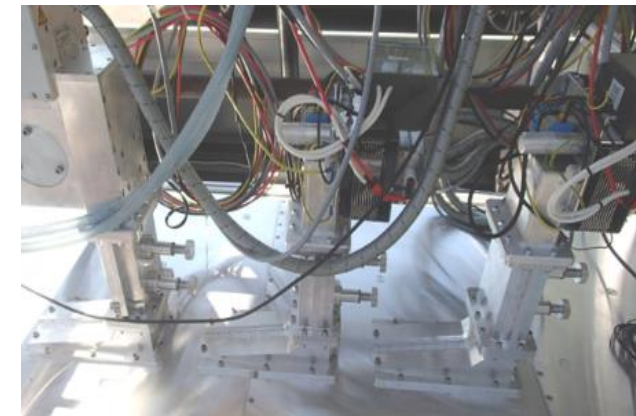
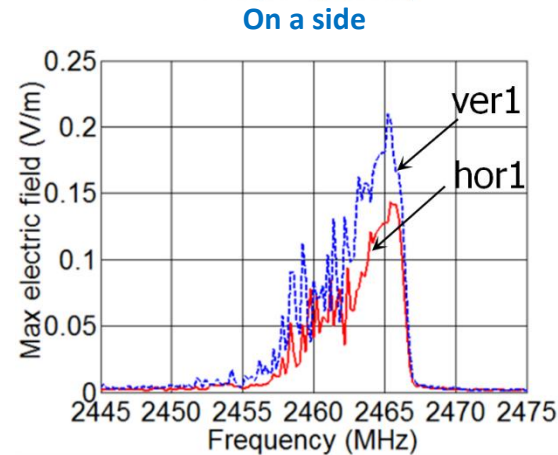
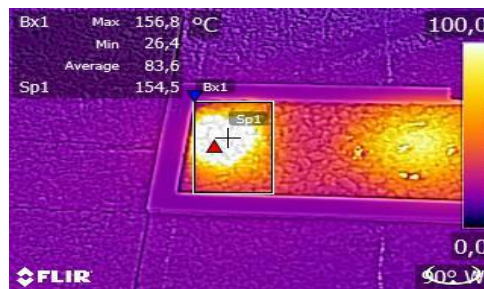
Simulated & measured reflection coefficient



Exposure levels @ 0.5m from applicator  
Below standardized limits



Measured temperature distribution

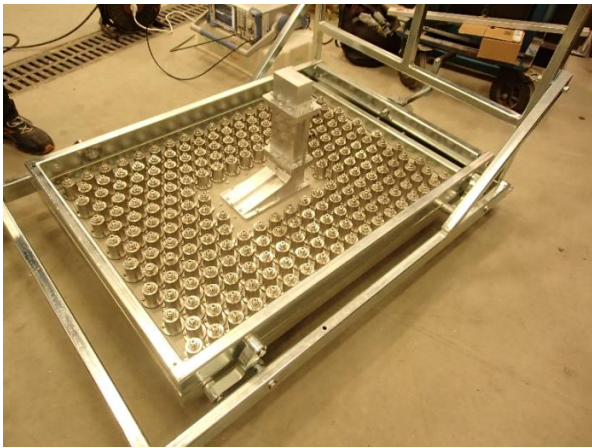
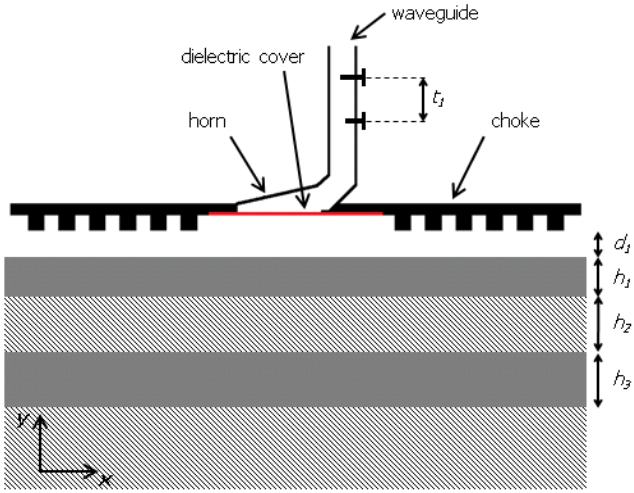


System of three MW power applicators with feeding system and leakage preventing chokes: designed, manufactured, tested

High power applicator with a system of chokes preventing  $\mu\text{W}$  energy leakage

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 regimes



Microwave applicator for thermal treatment of bituminous surfaces

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

Cambridge, 29-31 May 2019



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

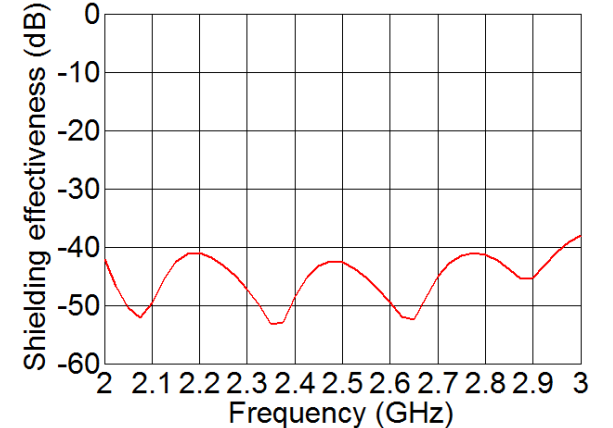
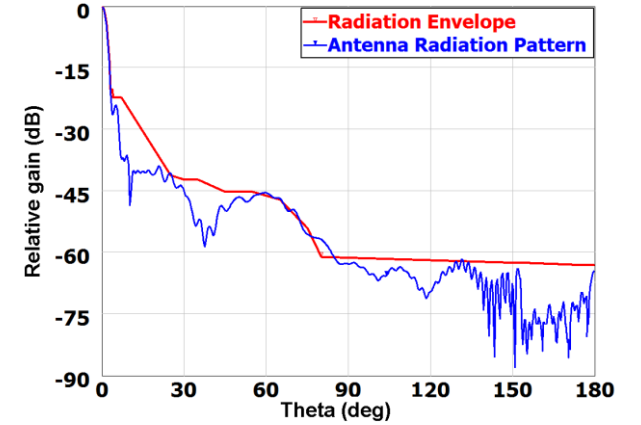
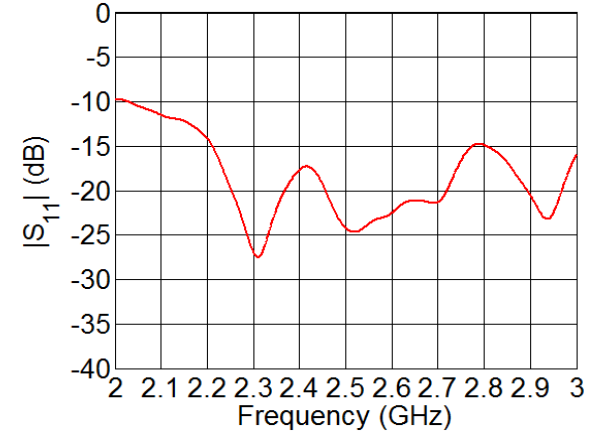


Simulation results saved to file

External application – objective extraction from file



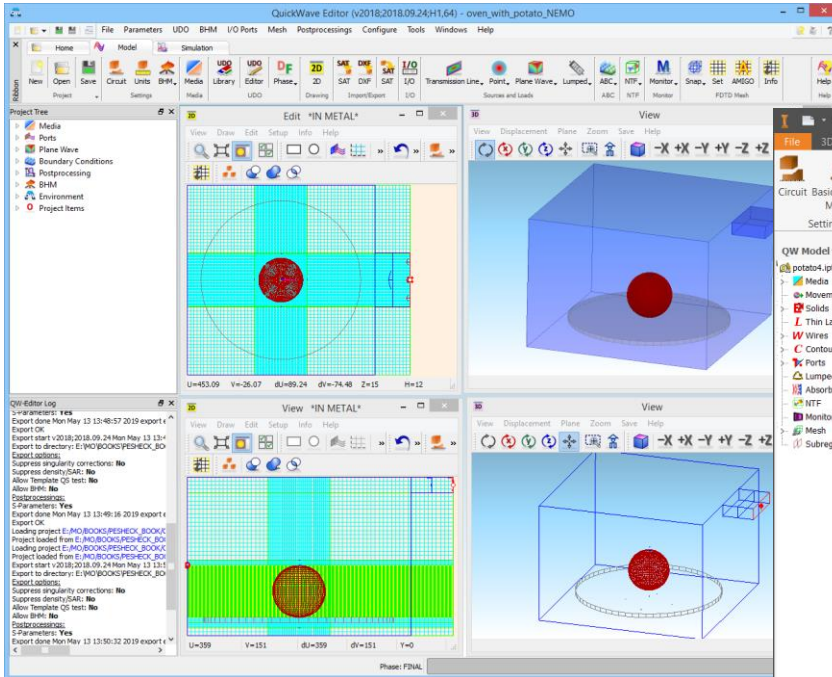
Optimiser – internal or external





# Dedicated user interfaces for parametrised project creation

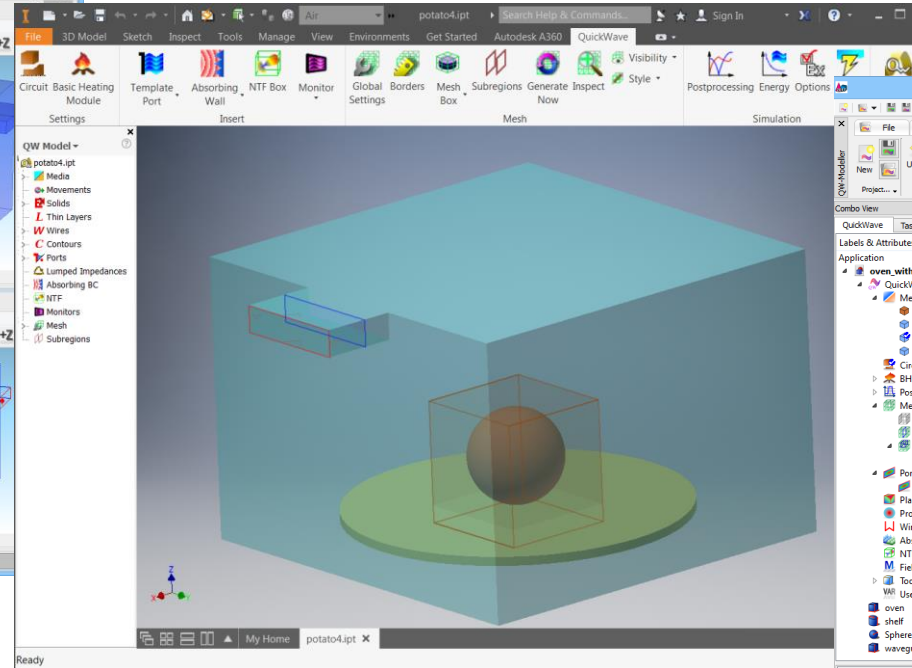
## QW-Editor



In-house, script based

Import/export to \*.sat & \*.dxf

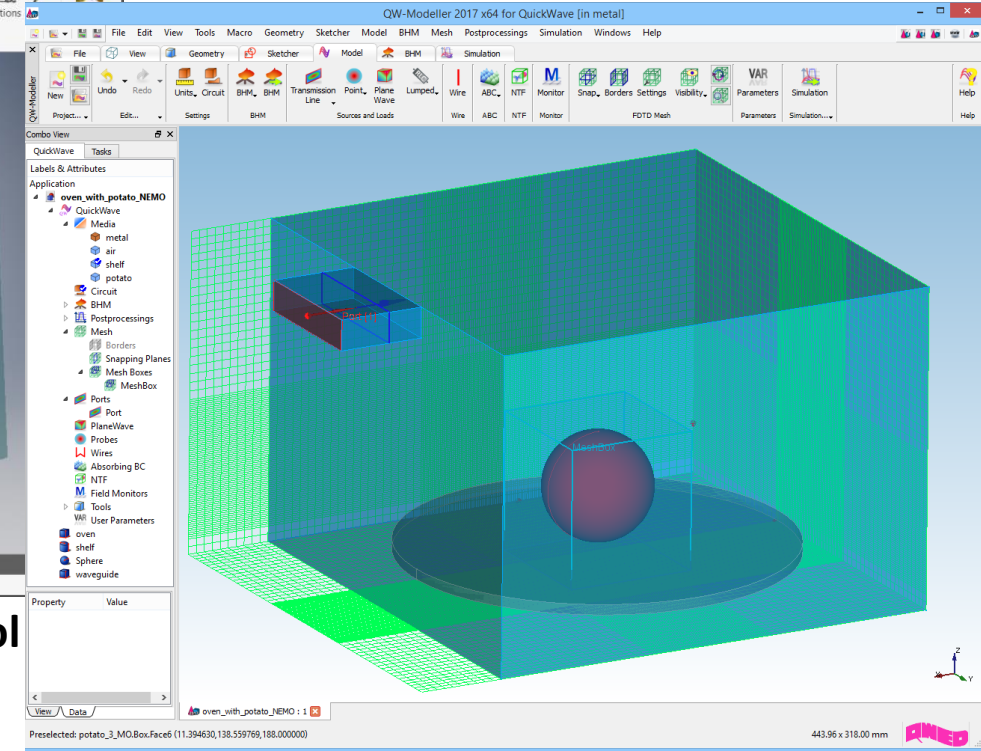
## QW-AddIn for Autodesk Inventor Software



Based on advanced professional CAD tool

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

## QW-Modeller



CAD tool - FreeCAD based

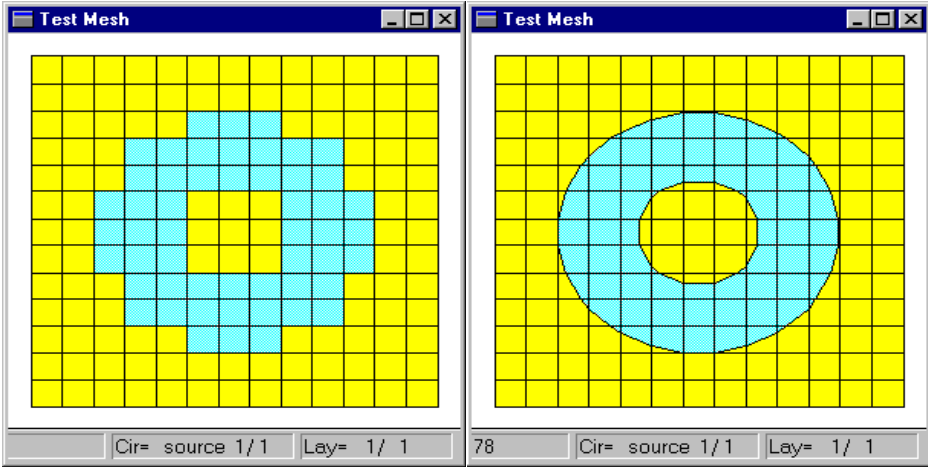
Free of charge, No licences, No time restrictions, No project limitations

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

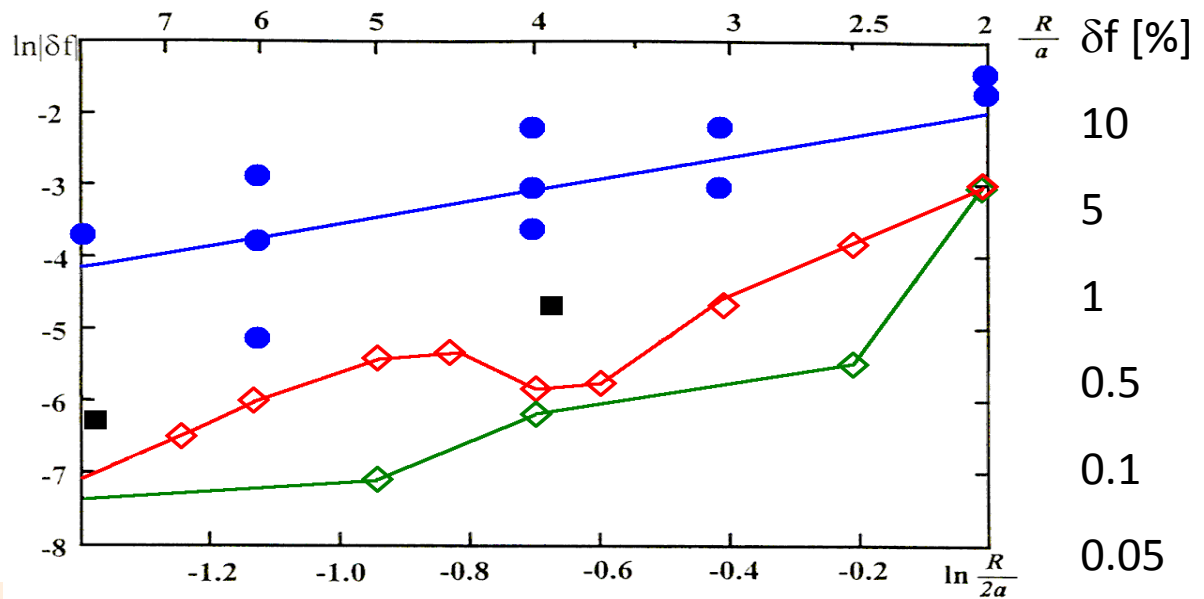
*Curiosity: export of CAD files from "old" QW-Editor for further manufacturing is reported by our user.*

# Conformal modelling of complex ovens & loads

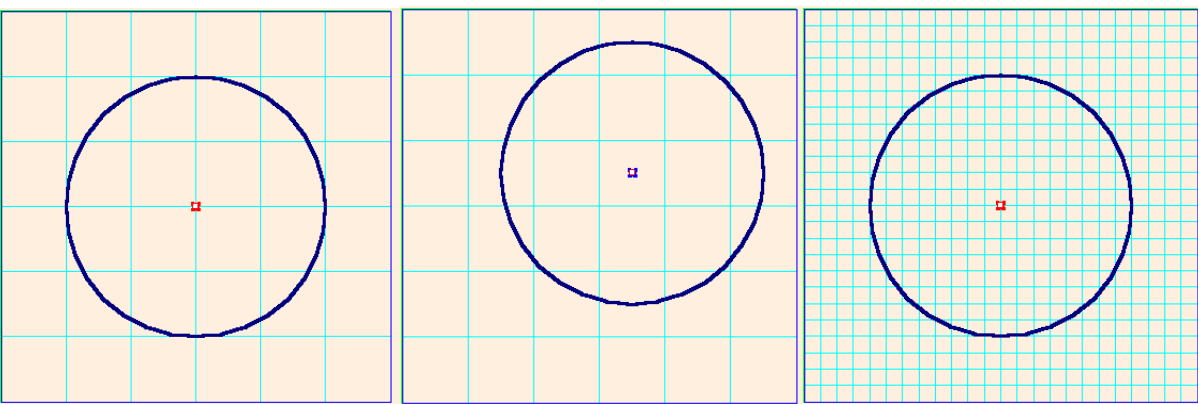
Recalling pre-published results on local conformal approximations



stair-case vs locally conformal mesh  
coax line, hot-dog, donut



stair-case  
no or simple merging (Railton & Schneider, *MTT Trans.* Jan1999)  
directional cell merging  
linearised directional cell merging

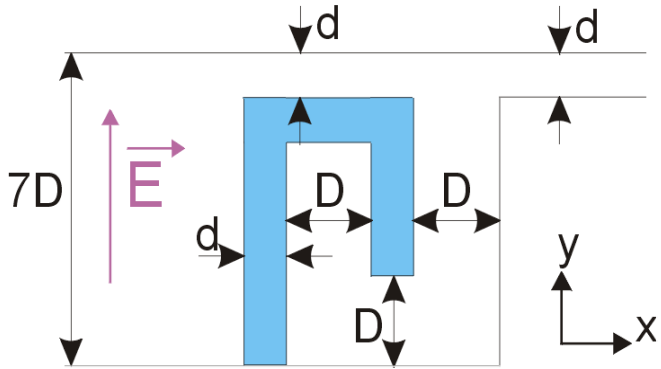


cross-section of: glass plate, pizza, cylindrical resonator  
mesh 2..8 cells per radius; results depend on object location vs mesh

Conformal 2D FDTD as originally proposed  
by W.Gwarek, *IEEE Trans. MTT* 1985, 1988  
Microwave Pioneer Award 2011

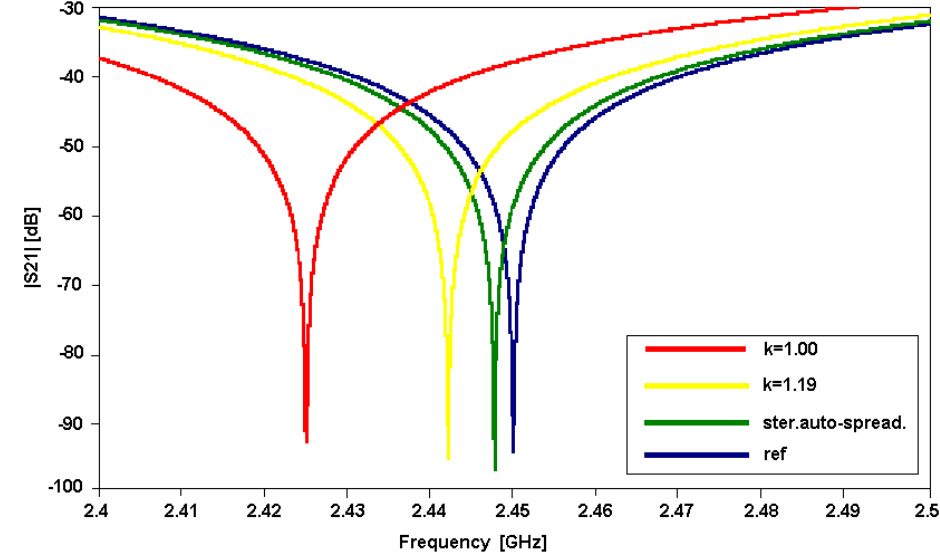
# Modelling of field singularities at sharp metal edges

Recalling pre-published results on local conformal approximations

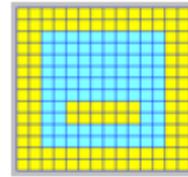


Choke of a MW oven in raw FDTD gives frequency error about 40x bigger than dispersion error.  
Proper model suppresses singularity error to dispersion error.

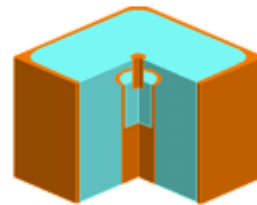
	errors by raw FD / FDTD	action by singularity models
$E$ -field	$\epsilon \uparrow$	$\epsilon \downarrow$
$H$ -field	$\mu \downarrow$	$\mu \uparrow$
$Z_0$	$\downarrow$	$\uparrow$
$f$	depends on mode	consider stability



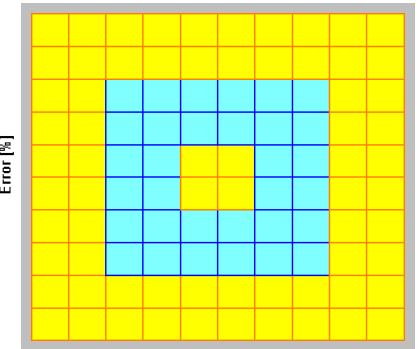
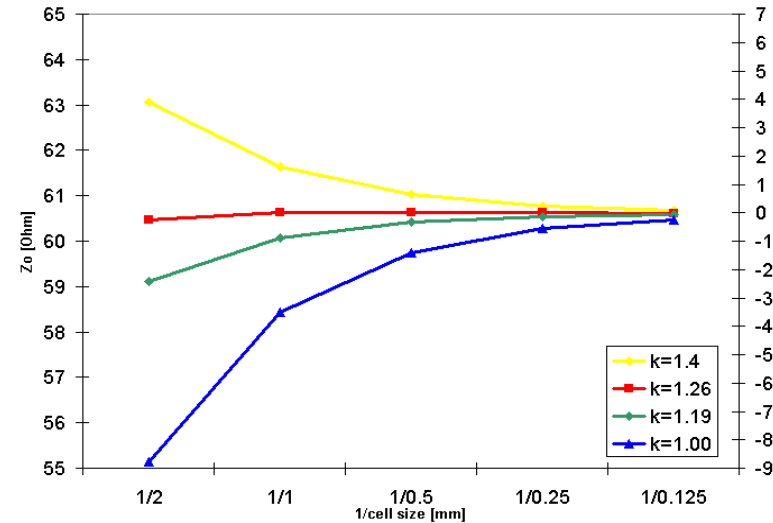
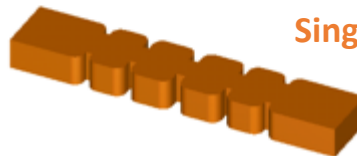
## TEM transmission lines



## resonators



## filters



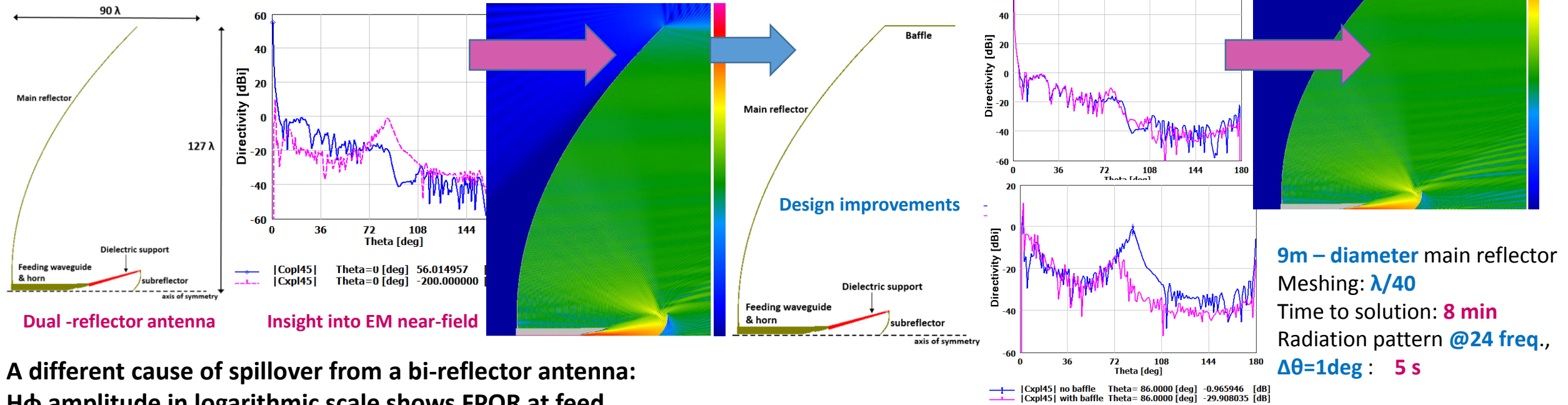
In TEM lines singularity errors of both field types boost the impedance error. Singularity corrections become indispensable for analysis at computer effort.

Stereoscopic singularity models  
M.Celuch *IEEE IMS* 2003

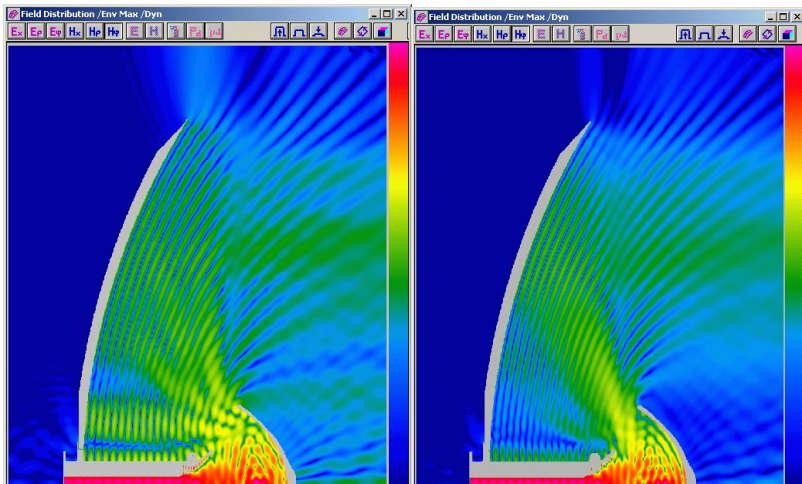


# Near-field insight into device performance

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

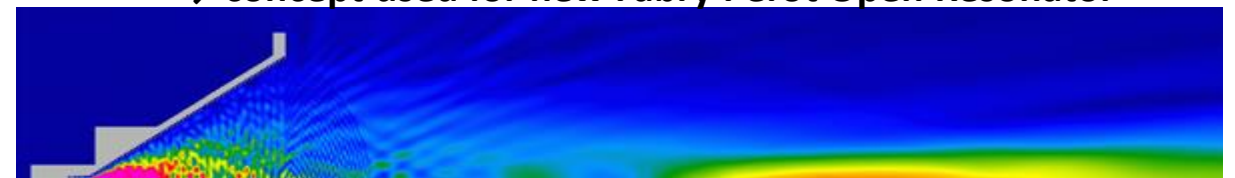


A different cause of spillover from a bi-reflector antenna:  
 H $\phi$  amplitude in logarithmic scale shows FPOR at feed  
 from max (purple) down to -60 dB (blue) at two freqs. within 3 %



Gaussian beam formation for quasi-free-space material measurements  
 → concept used for new Fabry Perot Open Resonator

## BOR FDTD



Scenarios modelled full-wave: **250 λ** (in each dir.) modelled on average laptop  
**2500 λ** on popular PC  
**5000 λ** on top-shelf PC



# Conclusions

- Electromagnetic modelling is a powerful tool for the development of new material measurement methods:
  - new test fixtures,
  - resolution improvement,
  - physical interpretation of the measured results.
- Measurements are not "universal truth"; they are subject to definitions & conventions, just like the modelling.
- EM modelling in general-purpose software helps bridging the gaps between seemingly different technology domains:
  - *near field imaging* explains exploding eggs *but also* helps in material measurements,
  - *Brewster angle* is exploited in telecommunications *but also* in domestic MW ovens.
- Modelling lies at the basis of material measurements,
- ...but modelling itself is only as good as the previously measured material parameters.
- Two approaches to commercial software development:
  - *black box* that quickly provides *solutions = numbers*,
  - *virtual laboratory* that provides *physical insight*.
- With this keynote I seek:
  - **advice** on matrix inversion in imaging,
  - reseach **collaborations** to explore & enrich QuickWave modelling.

## THANK YOU!