

# gprMax + MPI

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Large-scale open-source computational  
electrodynamics

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THE UNIVERSITY  
of EDINBURGH



Northumbria  
University  
NEWCASTLE

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# What is gprMax?



**"gprMax is a full-wave numerical modelling software package that is based on the finite-difference time-domain method for solving Maxwell's equations. It was initially developed to simulate the complex responses of ground penetrating radar systems."**

"gpr" from "ground penetrating radar" and "Max" from "Maxwell"

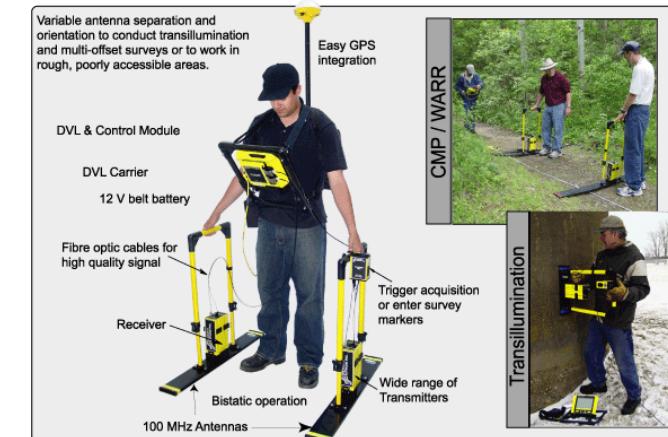
<https://www.gprmax.com>

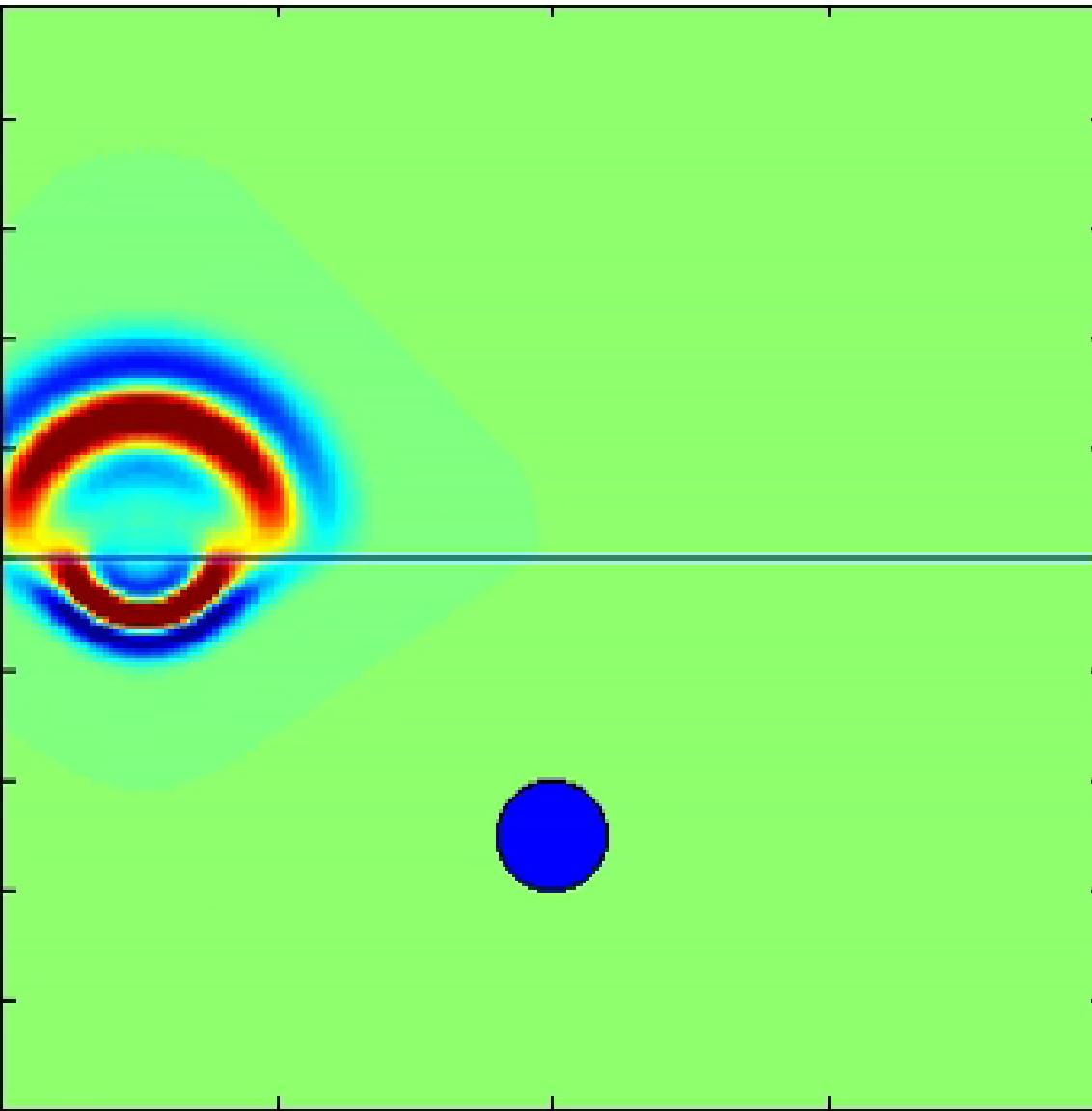
<https://github.com/gprmax/gprMax>

<http://docs.gprmax.com/en/latest/>

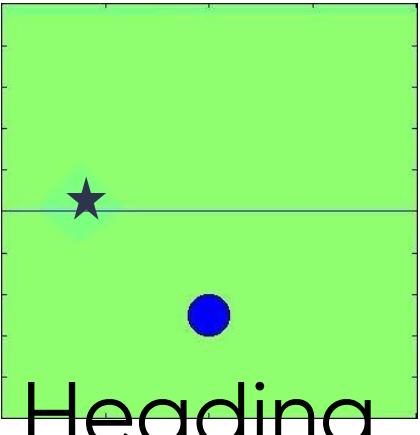
# What is GPR?

" ... a term that describes both a piece of equipment - an Ultra Wide Band Radar - and a method to investigate into opaque objects and gather useful information about their composition.."

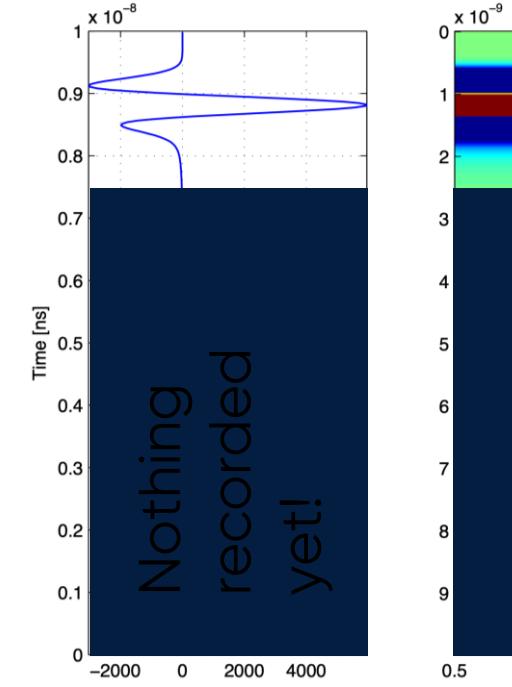
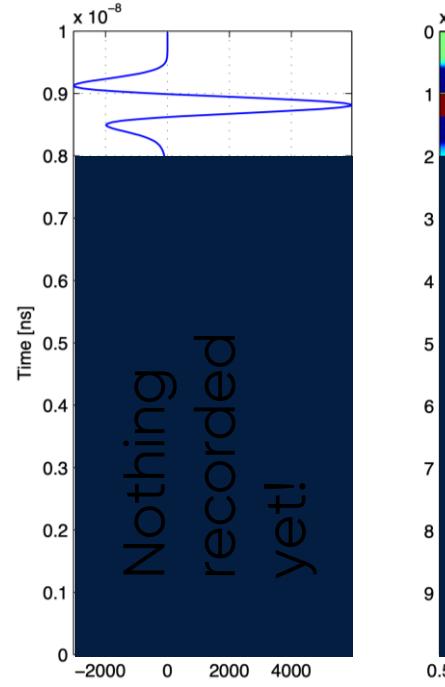
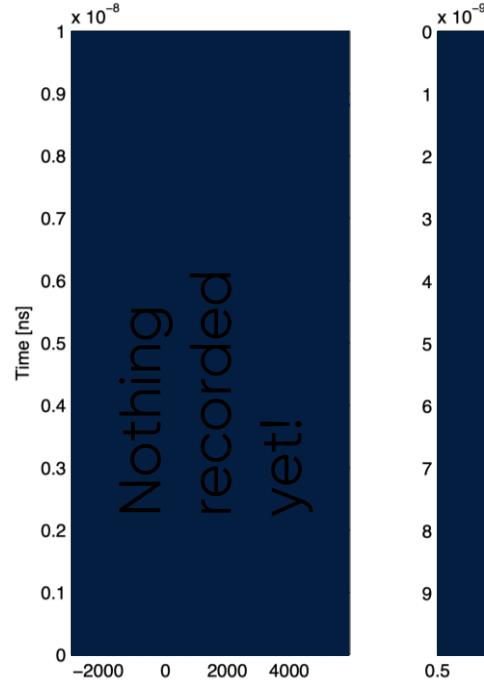
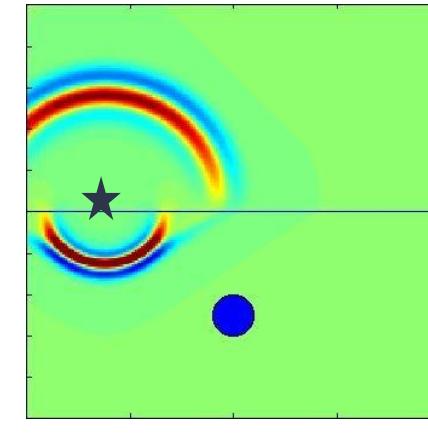
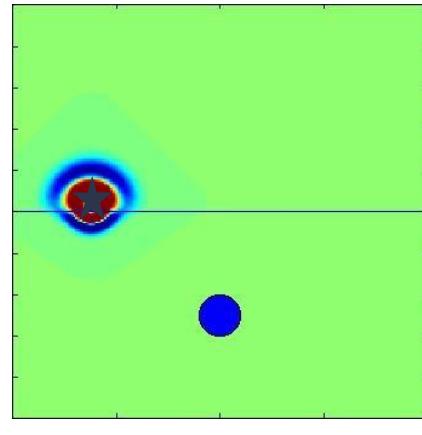


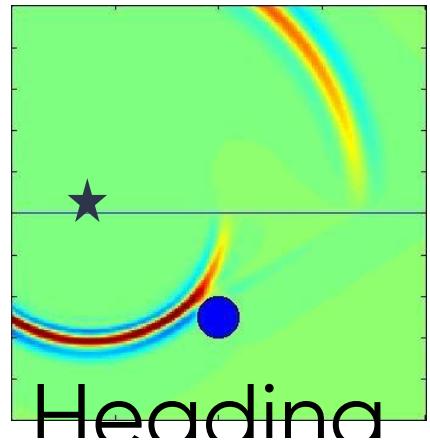


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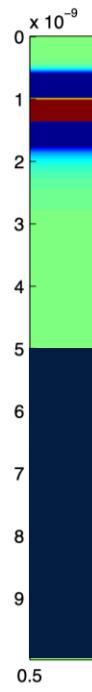
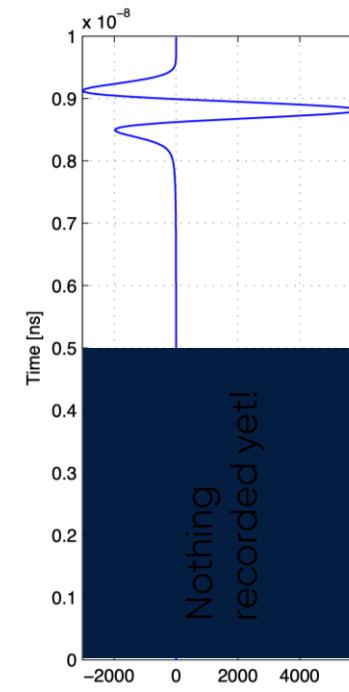
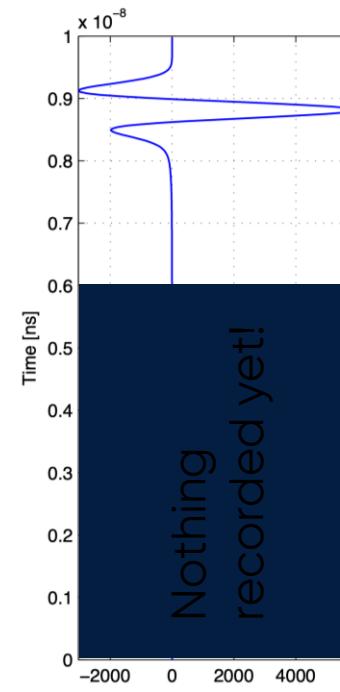
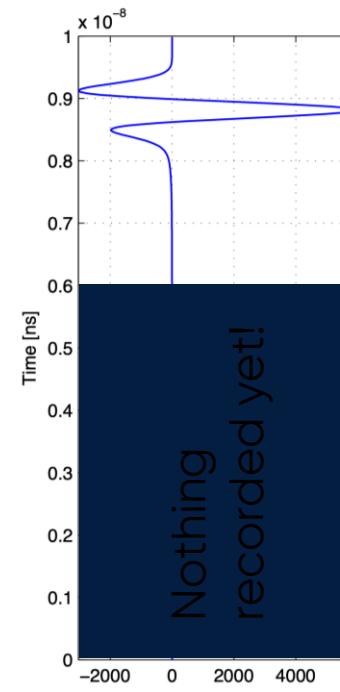
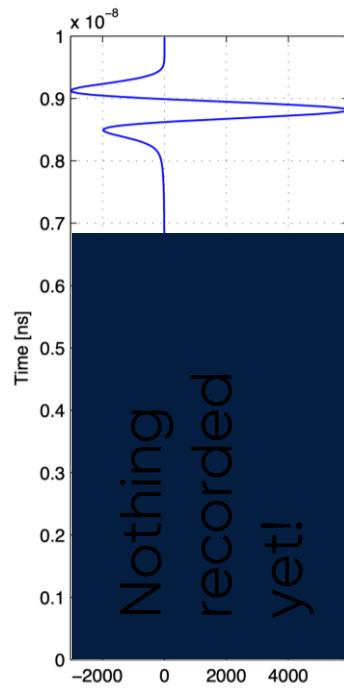
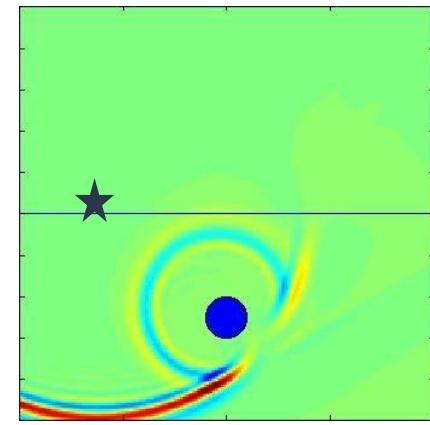
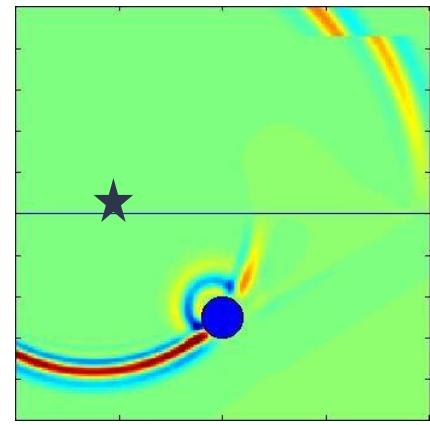


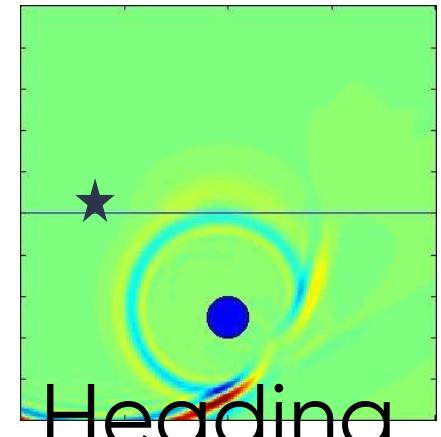
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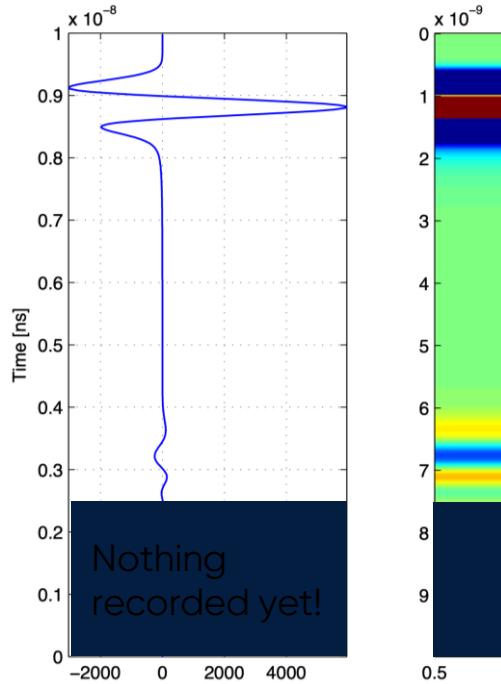
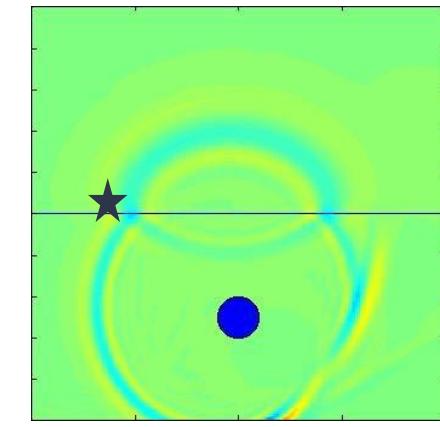
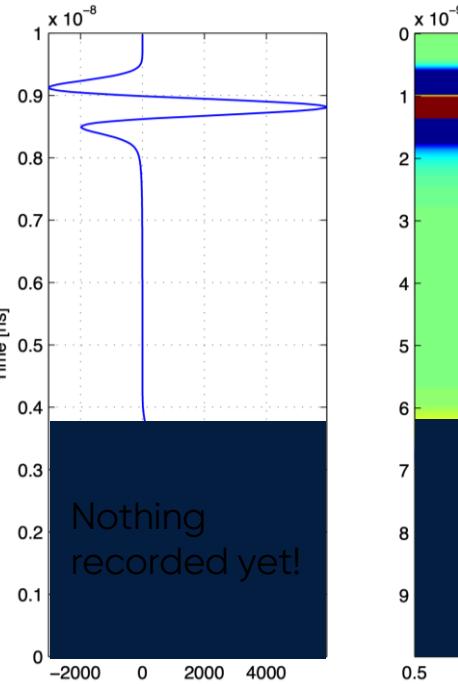
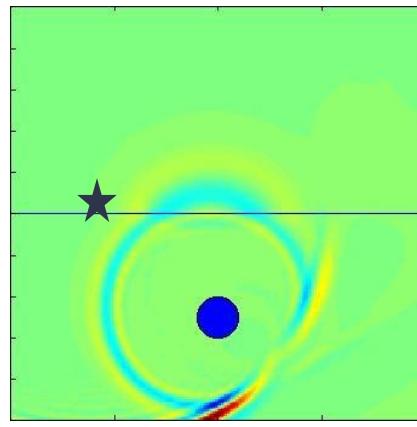
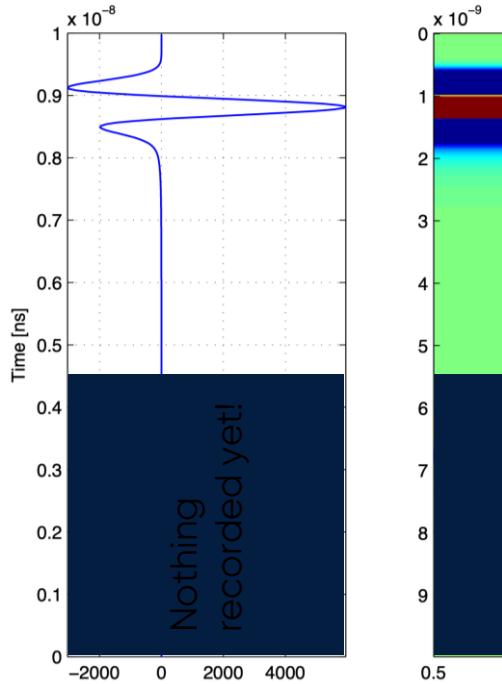


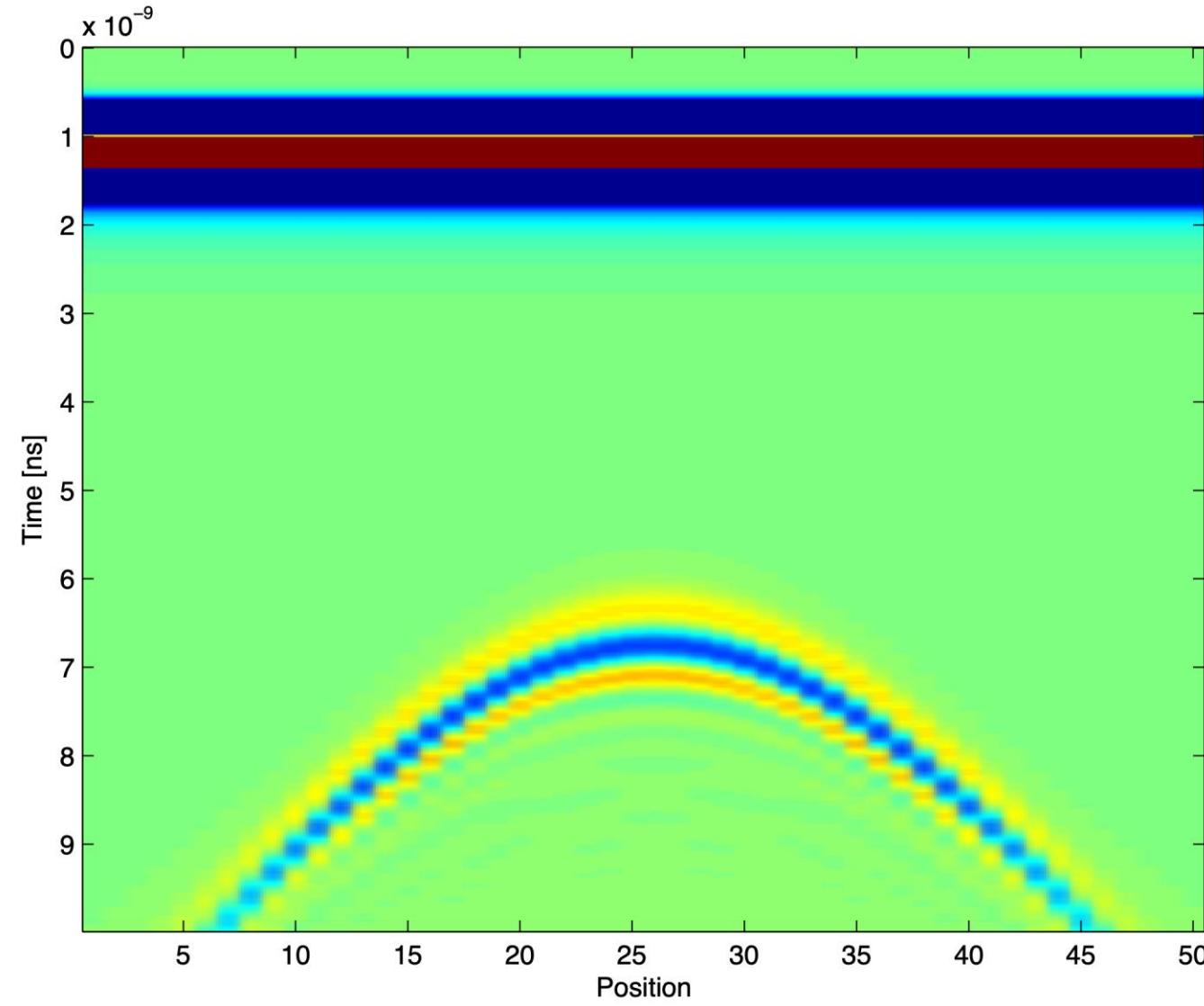
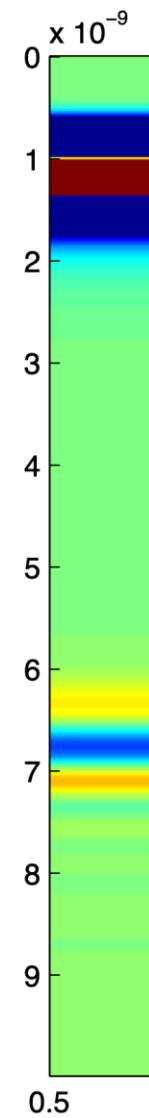
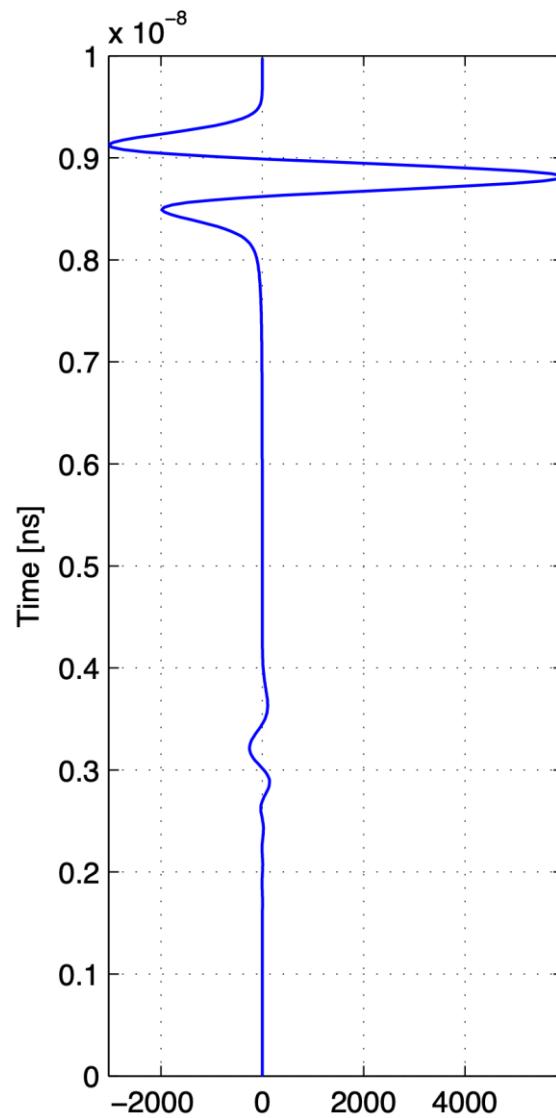
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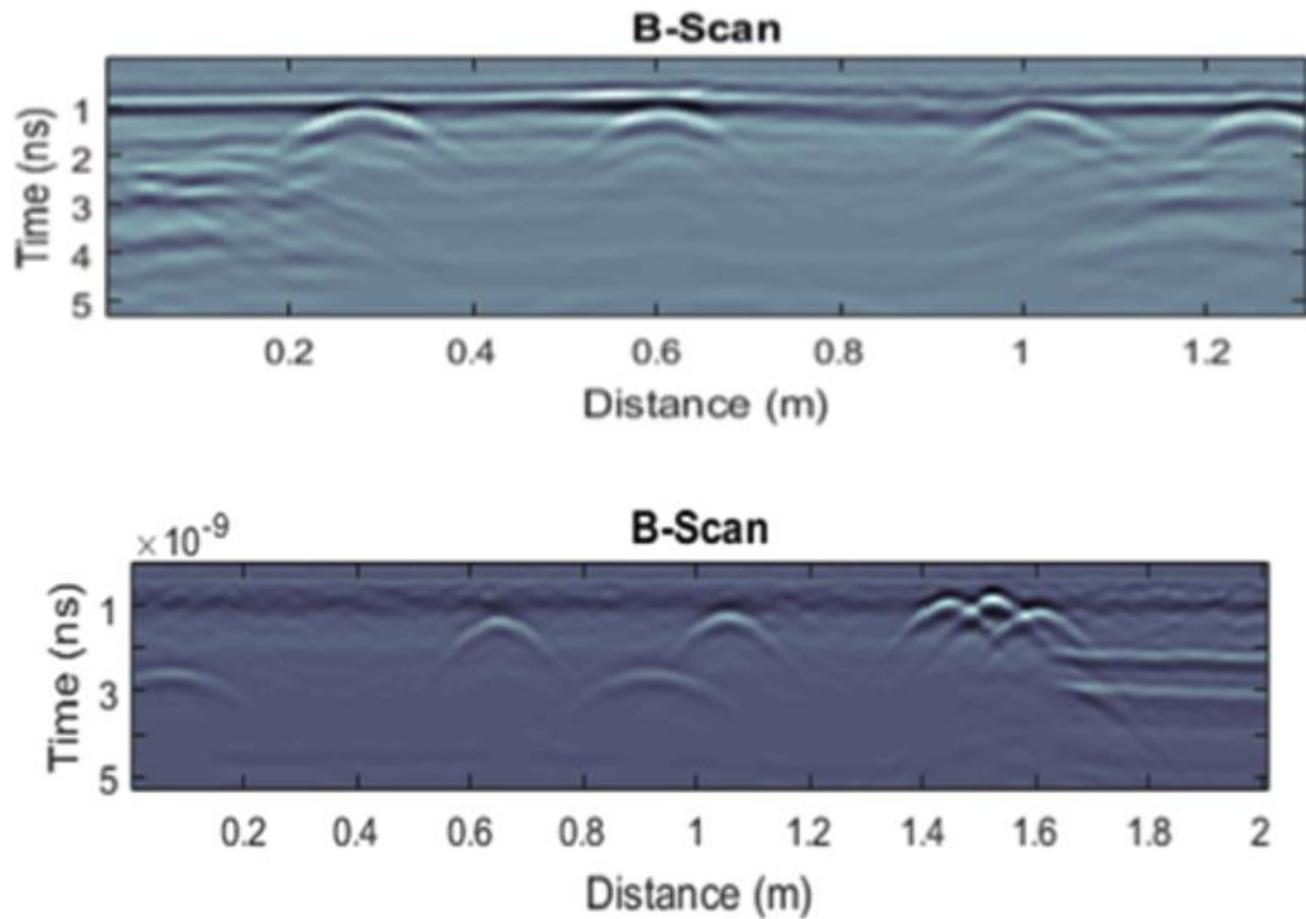
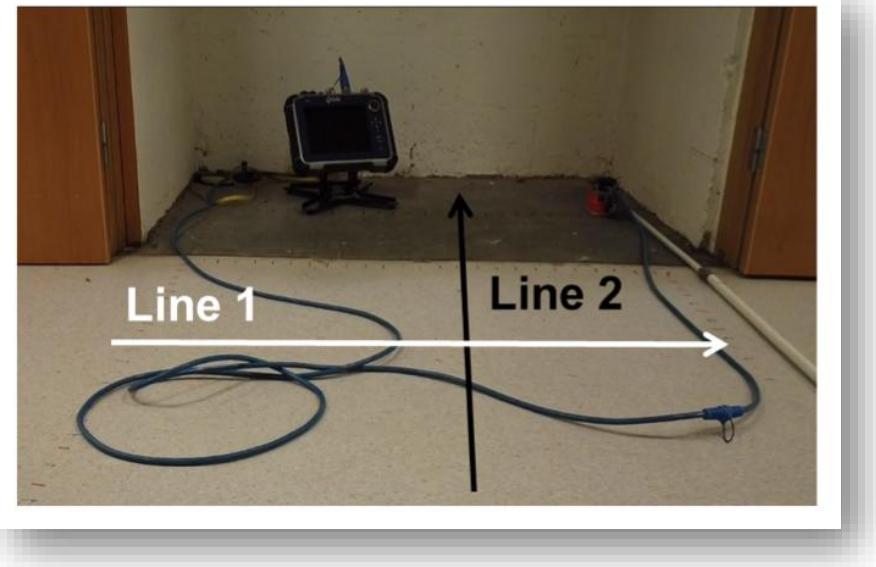




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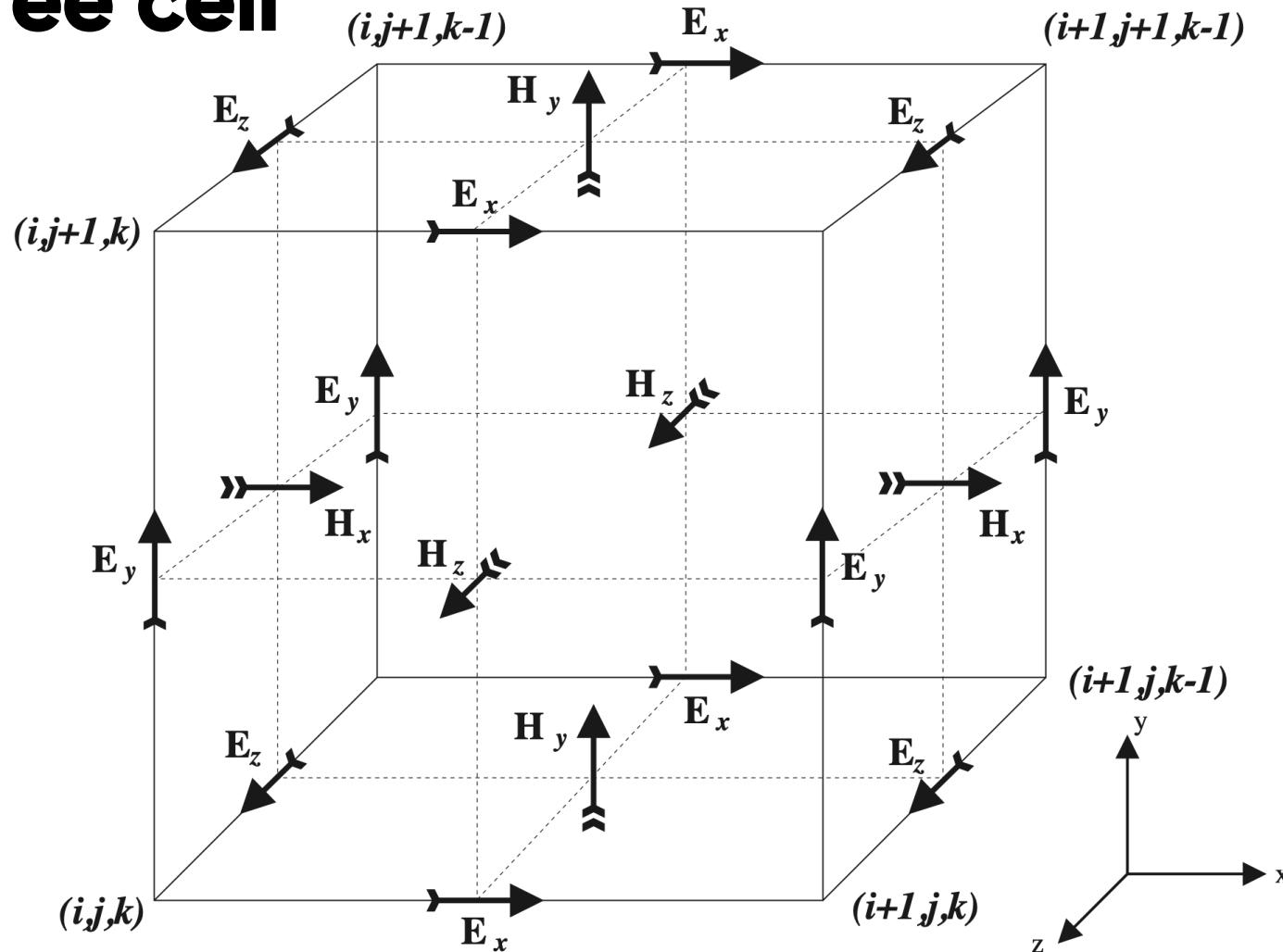
$$\oint_C \mathbf{E} \cdot d\hat{\mathbf{l}} = - \iint_S \frac{\partial \mathbf{B}}{\partial t} \cdot d\hat{\mathbf{s}}$$



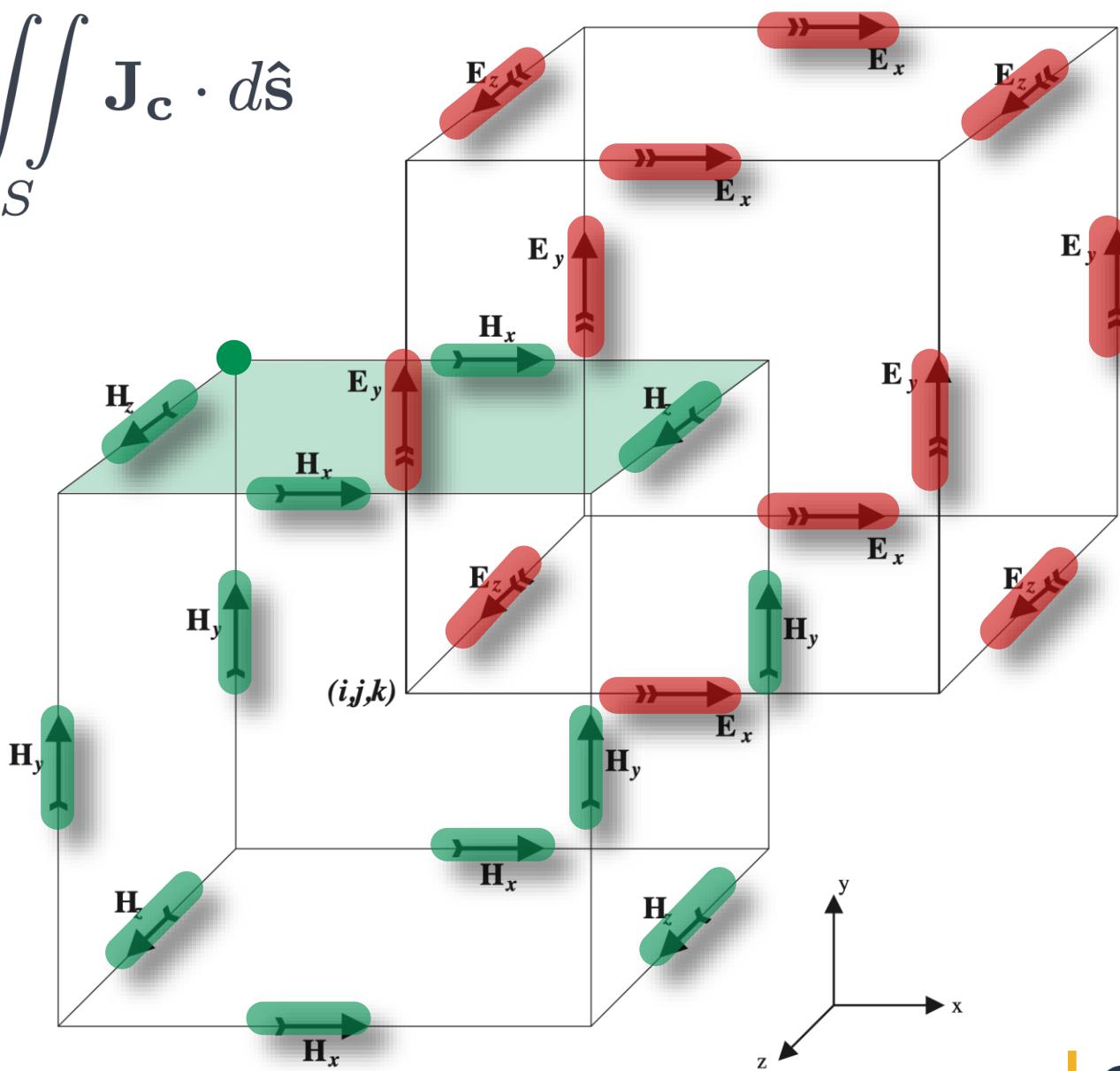
$$\oint_C \mathbf{H} \cdot d\hat{\mathbf{l}} = \iint_S \frac{\partial \mathbf{D}}{\partial t} \cdot d\hat{\mathbf{s}} + \iint_S \mathbf{J}_c \cdot d\hat{\mathbf{s}} + \iint_S \mathbf{J}_s \cdot d\hat{\mathbf{s}}$$

$$\iint_S \mathbf{D} \cdot d\hat{\mathbf{s}} = \iiint_V q dV \quad \iint_S \mathbf{B} \cdot d\hat{\mathbf{s}} = 0$$

# The FDTD Yee cell



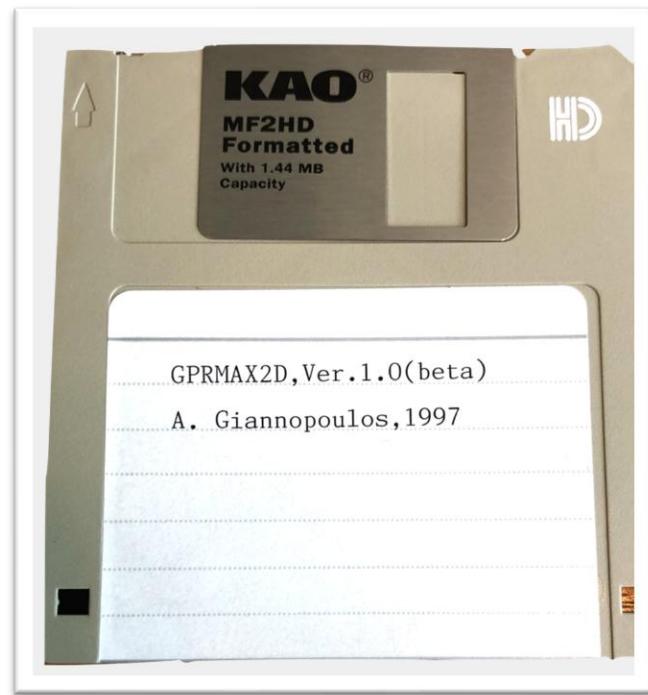
$$\oint_C \mathbf{H} \cdot d\hat{\mathbf{l}} = \iint_S \frac{\partial \mathbf{D}}{\partial t} \cdot d\hat{\mathbf{s}} + \iint_S \mathbf{J}_c \cdot d\hat{\mathbf{s}}$$



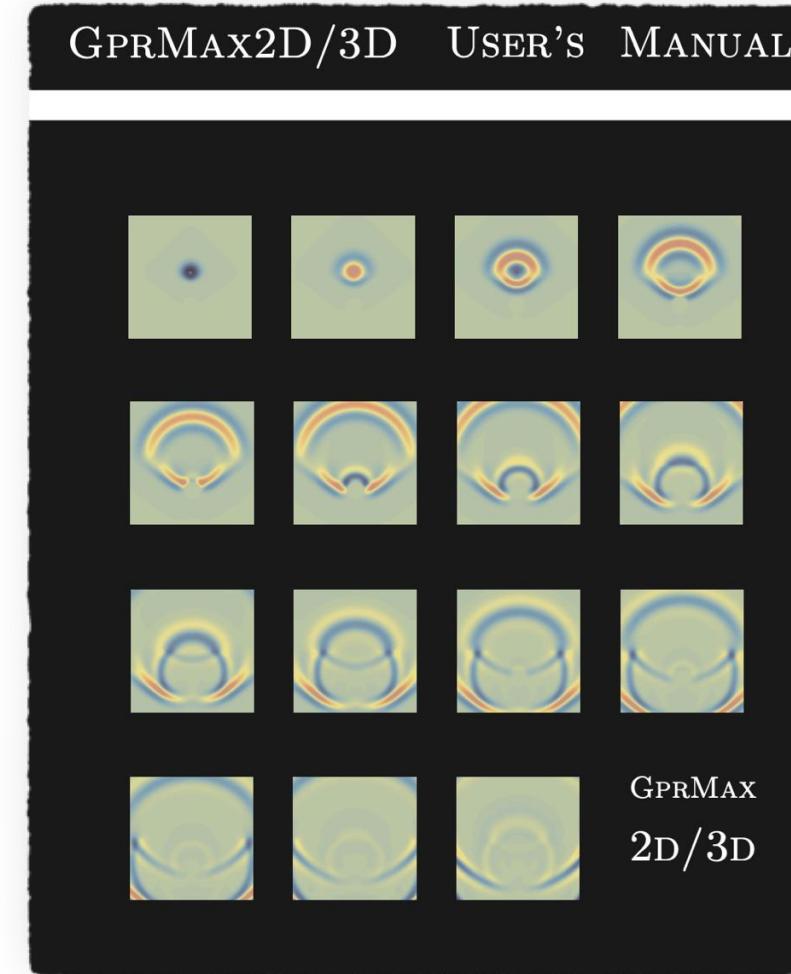
# A short history of gprMax

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# 1997



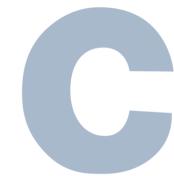
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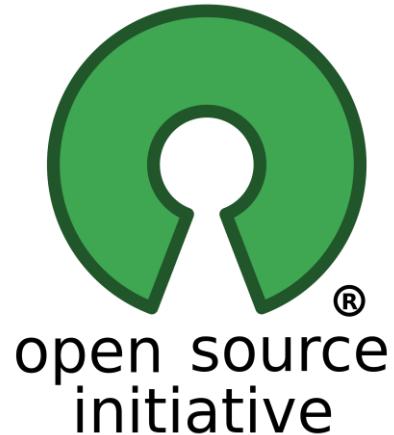
# 2015

The screenshot shows the 'gprMax User Guide' documentation. The left sidebar contains navigation links for 'INTRODUCTION', 'USING GPRMAX', 'PYTHON TOOLS', 'ADVANCED TOPICS', 'USER LIBRARIES', and 'GPGPU'. The main content area features the title 'gprMax User Guide' and a section titled 'Introduction' with a list of topics. To the right of the text are icons for 'HTML' (an orange '5' inside a red shield), 'ePUB' (a green 'e' inside a green square), and 'PDF' (a white document with a red 'PDF' label).



This screenshot shows a GitHub release page for 'v.3.0.0 (Bowmore)'. The page includes a release date of 'Jun 7, 2016', the author 'craig-warren', and the commit hash 'v.3.0.0 88b847c'. A 'Compare' button is also visible. The main content highlights the features of version 3.0.0, such as anisotropic material modelling, dispersive material modelling, and modelling of soils. It also mentions building of heterogeneous objects and rough surfaces, and built-in libraries of antenna models. Links to the User Guide and Google Group forum are provided at the bottom.

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ELSEVIER

**gprMax: Open source software to simulate electromagnetic wave propagation for Ground Penetrating Radar\***

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Ground Penetrating Radar  
Finite-Difference Time-Domain  
Open source  
Python

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**ABSTRACT**

gprMax is open source software that simulates electromagnetic wave propagation, using the Finite-Difference Time-Domain (FDTD) method, for the numerical modelling of Ground Penetrating Radar (GPR). gprMax was originally developed in 1996 when numerical modelling using the FDTD method and, in general, the numerical modelling of GPR were in their infancy. Current computing resources offer the opportunity to build detailed and complex FDTD models of GPR to an extent that was not previously possible. To enable these types of simulations to be more easily realised, and also to facilitate the addition of more advanced features, gprMax has been redeveloped and significantly modernised. The original C-based code has been completely rewritten using a combination of Python and Cython programming languages. Standard and robust file formats have been chosen for geometry and field output files. New advanced modelling features have been added including: an unsplit implementation of higher order Perfectly Matched Layers (PMLs) using a recursive integration approach; diagonally anisotropic materials; dispersive media using multi-pole Debye, Drude or Lorenz expressions; soil modelling using a semi-empirical formulation for dielectric properties and fractals for geometric characteristics; rough surface generation; and the ability to embed complex transducers and targets.



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# 2017



Jun 19, 2017  
craig-warren  
v.3.1.0  
3c8e5ba

[Compare](#)

## v.3.1.0 (Big Smoke)

This is the v.3.1.0, codenamed **Big Smoke**, release of gprMax.

It continues our whisky-based naming, and is also a reference to the cities of Edinburgh (Scotland) and San Francisco (USA). Why? Because the development of v.3.1.0 was funded, through a research project, by Google.

The most significant feature of this release is the ability for simulations to utilise **general-purpose computing using graphics processing units (GPGPU)**. We have used **NVIDIA's Compute-Unified Device Architecture (CUDA)**. Our testing on both consumer and data centre NVIDIA GPU cards has shown dramatic performance increases over our parallelised CPU (OpenMP) implementation.

You can read about how to use the GPU functionality and find all the features of gprMax described in detail in the User Guide (<http://docs.gprmax.com>)

Please report any bugs with code via Issues on GitHub.

For general help and questions about using gprMax visit our Google Group forum (<http://www.gprmax.com/forum.shtml>)

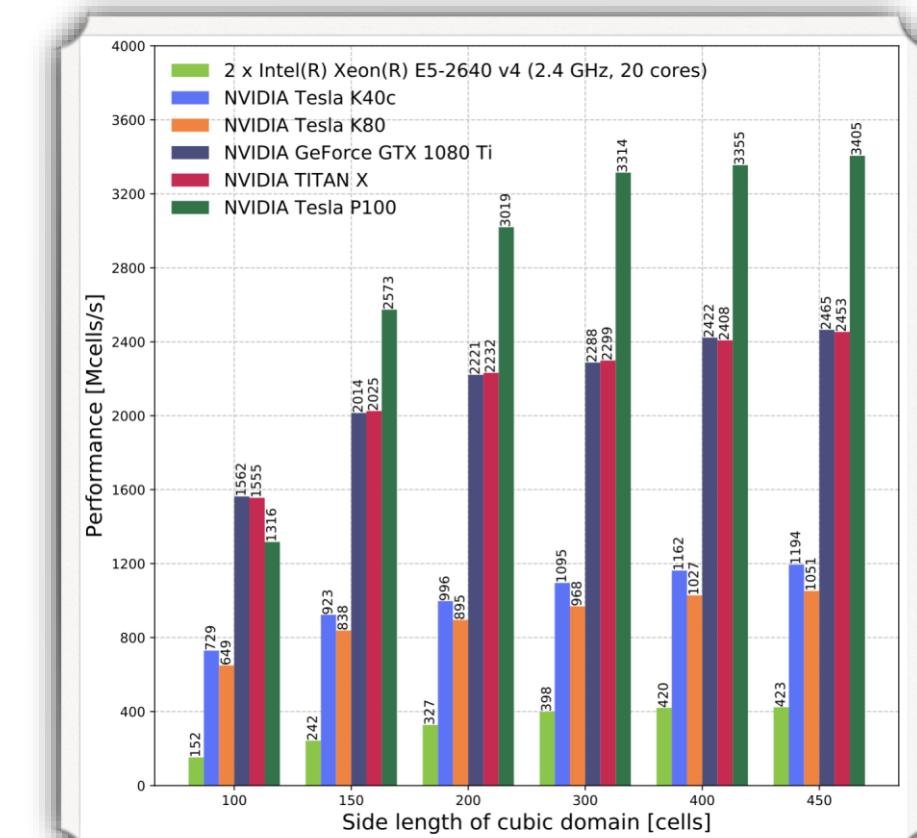
▶ Assets 2



Google



*Free as in Freedom*

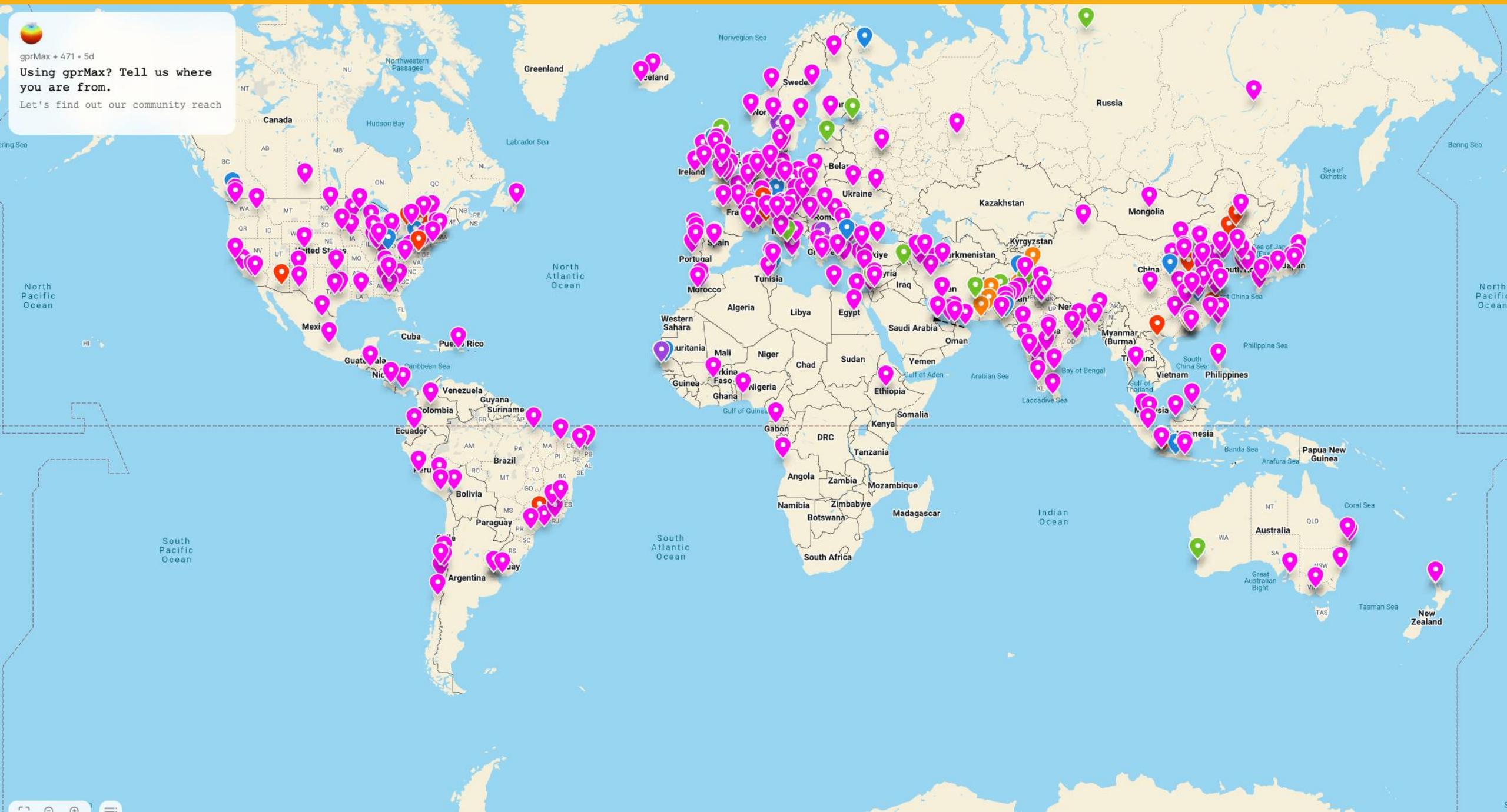


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gprMax + 471 + 5d

Using gprMax? Tell us where you are from.  
Let's find out our community reach



## Publications

### Cite gprMax

If you use gprMax and publish your work we would be grateful if you could cite our work!

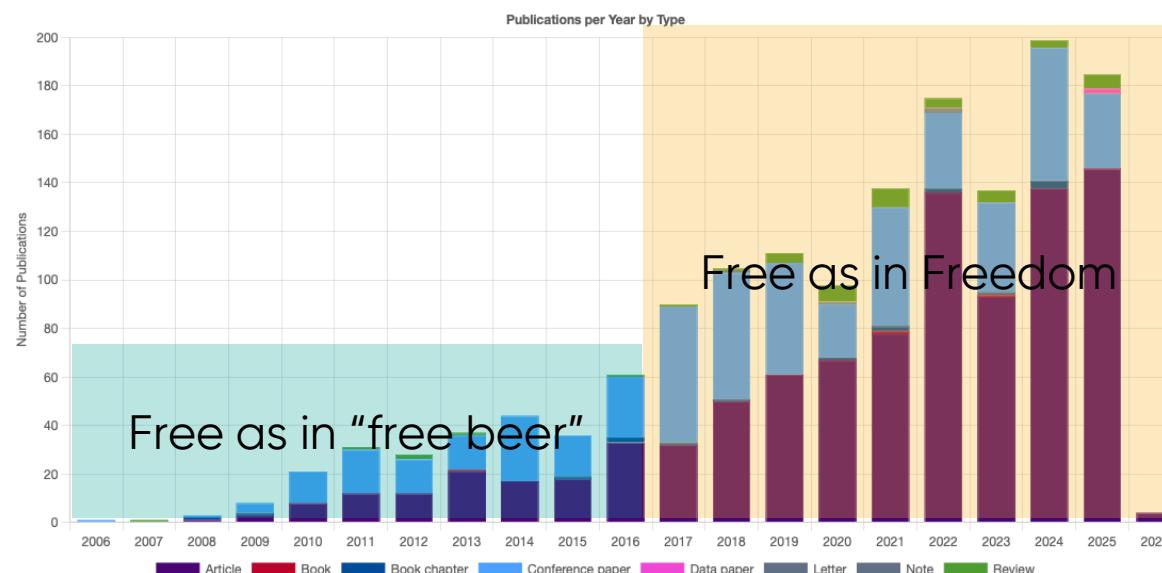
The principal reference for gprMax is [1] which describes the new version of the software and its main features. If you have used specific elements of the software you might also like to cite: [2] - GPU accelerated solver, [3] - soil modelling, rough surfaces; [4] - dispersive materials; [5] - advanced features of the RIPML; [6, 7] - GPR antenna models. If you wish to reference the development history of gprMax you can also cite [8].

1. Warren, C., Giannopoulos, A., & Giannakis, I. (2016). gprMax: Open source software to simulate electromagnetic wave propagation for Ground Penetrating Radar. *Computer Physics Communications*, 209, 163-170, [10.1016/j.cpc.2016.08.020](https://doi.org/10.1016/j.cpc.2016.08.020).
2. Warren, C., Giannopoulos, A., Gray, A., Giannakis, I., Patterson, A., Wetter, L., & Hamrah, A. (2018). A CUDA-based GPU engine for gprMax: Open source FDTD electromagnetic simulation software. *Computer Physics Communications*, 237, 208-218, [10.1016/j.cpc.2018.11.007](https://doi.org/10.1016/j.cpc.2018.11.007).
3. Giannakis, I., Giannopoulos, A., Warren, C. (2016). A Realistic FDTD Numerical Modeling Framework of Ground Penetrating Radar for Landmine Detection. *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, 9(1), 37-51, [10.1109/JSTARS.2015.2468597](https://doi.org/10.1109/JSTARS.2015.2468597).
4. Giannakis, I., Giannopoulos, A. (2014). A Novel Piecewise Linear Recursive Convolution Approach for Dispersive Media Using the Finite-Difference Time-Domain Method. *IEEE Transactions on Antennas and Propagation*, 62(5), 2669-2678, [10.1109/TAP.2014.2308549](https://doi.org/10.1109/TAP.2014.2308549).
5. Giannopoulos, A. (2012). Unsplit Implementation of Higher Order PMLs. *IEEE Transactions on Antennas and Propagation*, 60(3), 1479-1485, [10.1109/TAP.2011.2180344](https://doi.org/10.1109/TAP.2011.2180344).
6. Warren, C., Giannopoulos, A. (2011). Creating finite-difference time-domain models of commercial ground-penetrating radar antennas using Taguchi's optimization method. *Geophysics*, 76(2), G37-G47, [10.1190/1.3548506](https://doi.org/10.1190/1.3548506).
7. Giannakis, I., Giannopoulos, A., Warren, C. (2018). Realistic FDTD GPR antenna models optimised using a novel linear/non-linear Full Waveform Inversion. *IEEE Transactions on Geoscience & Remote Sensing*, 207(3), 1768-1778, [10.1109/TGRS.2018.2869027](https://doi.org/10.1109/TGRS.2018.2869027).
8. Giannopoulos, A. (2005). Modelling ground penetrating radar by GprMax. *Construction and Building Materials*, 19(10), 755-762, [10.1016/j.conbuildmat.2005.06.007](https://doi.org/10.1016/j.conbuildmat.2005.06.007).

You can also get [references](#) and links to the PhD theses of the development team.

### Research using gprMax

gprMax has been successfully used for a diverse range of applications in academia and industry, from fields including **engineering**, **geophysics**, **archaeology**, and **medicine**. The following table lists publications (extracted from [Scopus](#) on 23-11-2025) that have cited references [1], [2] and [8] excluding any self-citations of the authors.



# Basic capabilities

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# Our own Recursive integration perfectly matched layer (PML) implementation for higher order and multipole PMLs

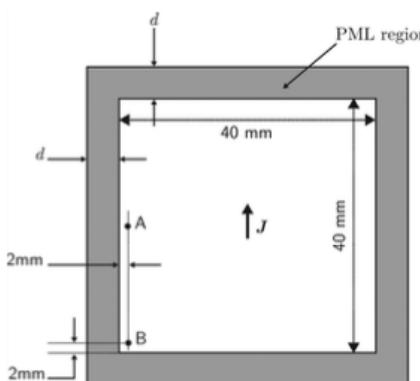
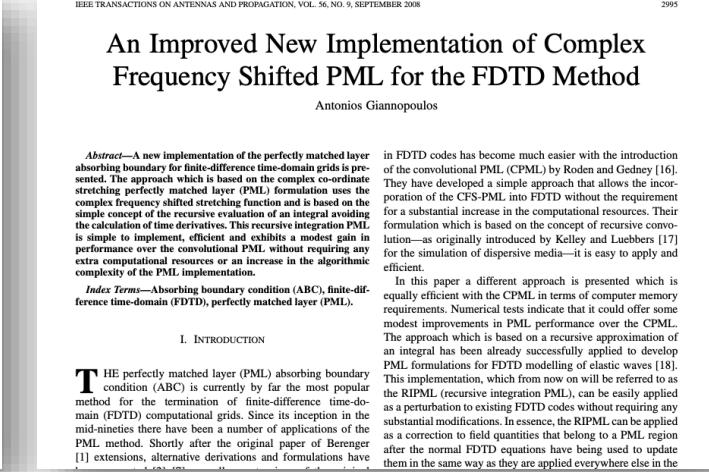
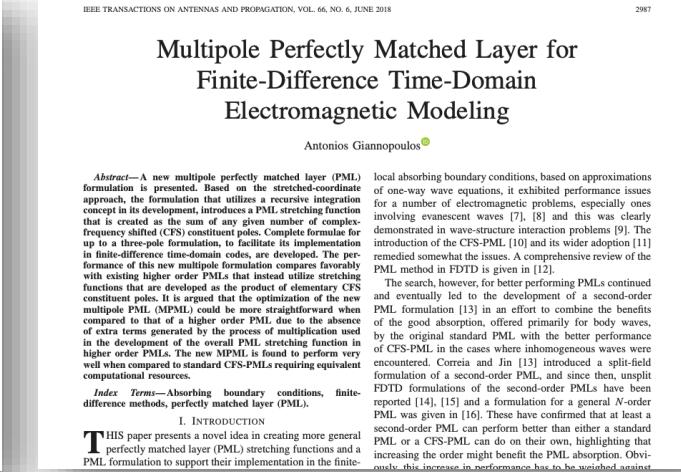
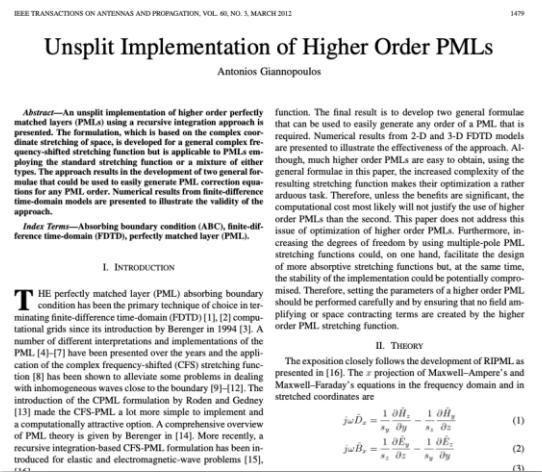


Fig. 1. Model of a y-directed electric current source at the centre of a  $40 \times 1$  mm cell  $TE_z$  FDTD grid. The computational domain is surrounded by a PML of thickness  $d$ . The  $E_y$  fields are sampled at points A and B [20, Ch. 7].

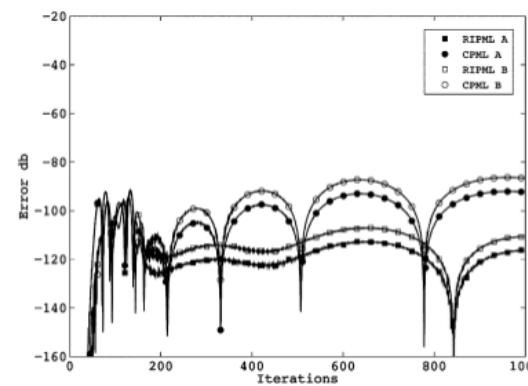


Fig. 3. Error in the  $E_z$  field component at points A and B for models terminated using RIPML and CPML.  $\kappa_{\max} = 1$  and  $\alpha_{\max} = 0.2$ .

# Our own very accurate dispersive media model

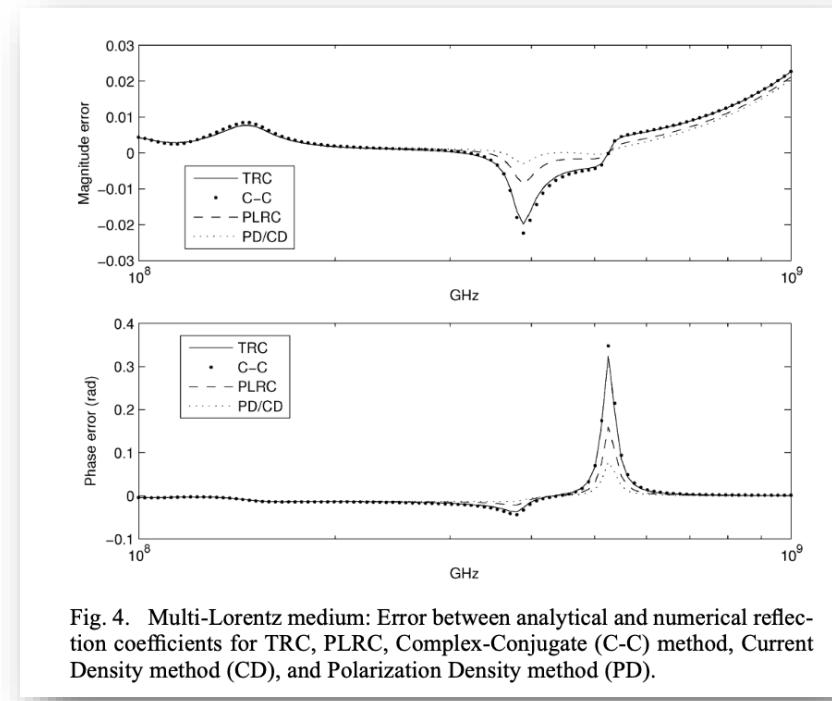
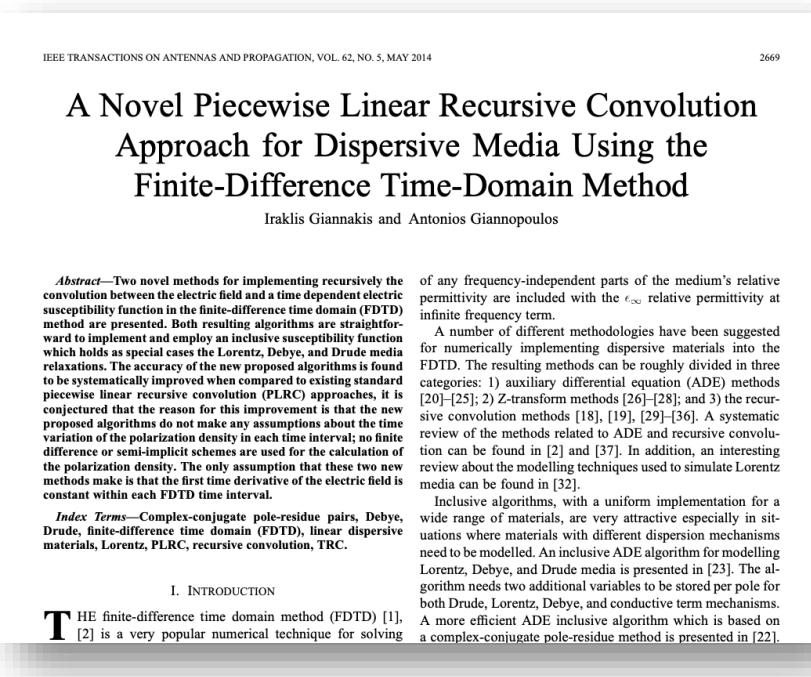


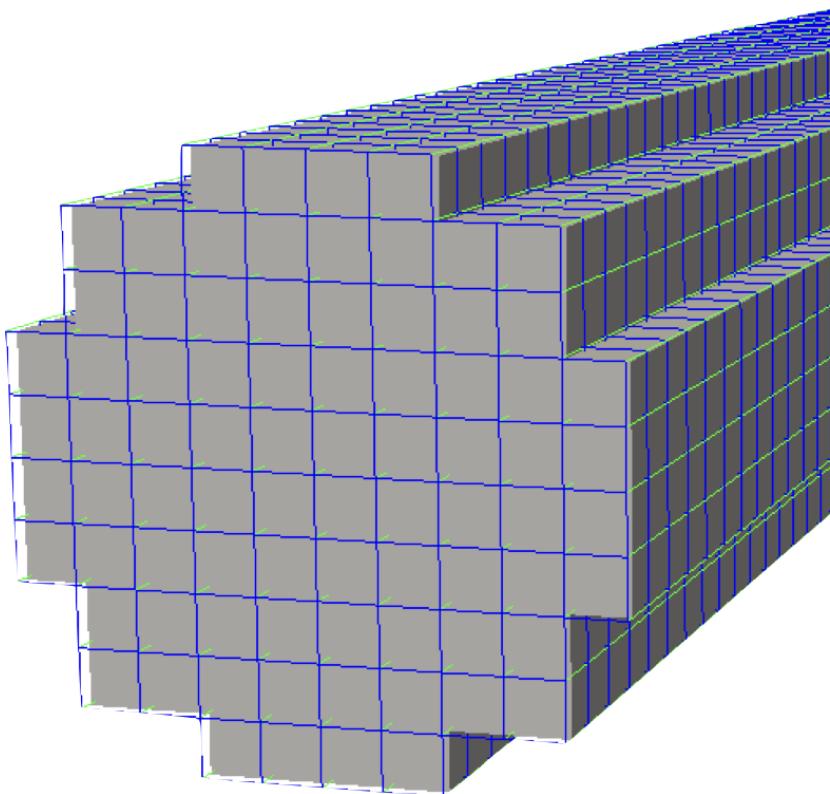
Fig. 4. Multi-Lorentz medium: Error between analytical and numerical reflection coefficients for TRC, PLRC, Complex-Conjugate (C-C) method, Current Density method (CD), and Polarization Density method (PD).

**Multi Debye, Drude and Lorentz materials and functionality that allows you to fit using multiple Debye poles arbitrary complex permittivity data**

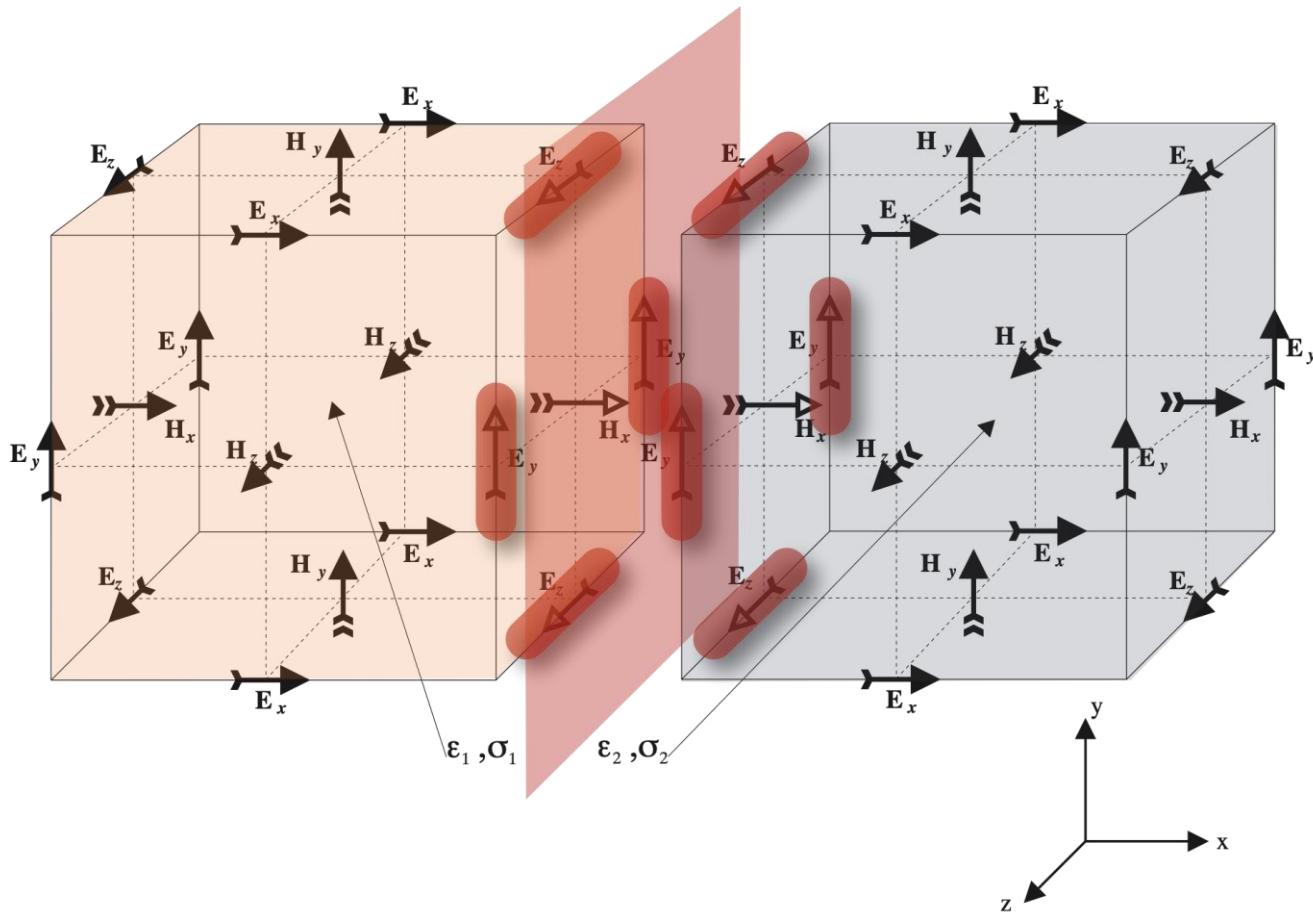
## Diagonally anisotropic materials

$$\bar{\epsilon} = \begin{bmatrix} \epsilon_{xx} & 0 & 0 \\ 0 & \epsilon_{yy} & 0 \\ 0 & 0 & \epsilon_{zz} \end{bmatrix}$$

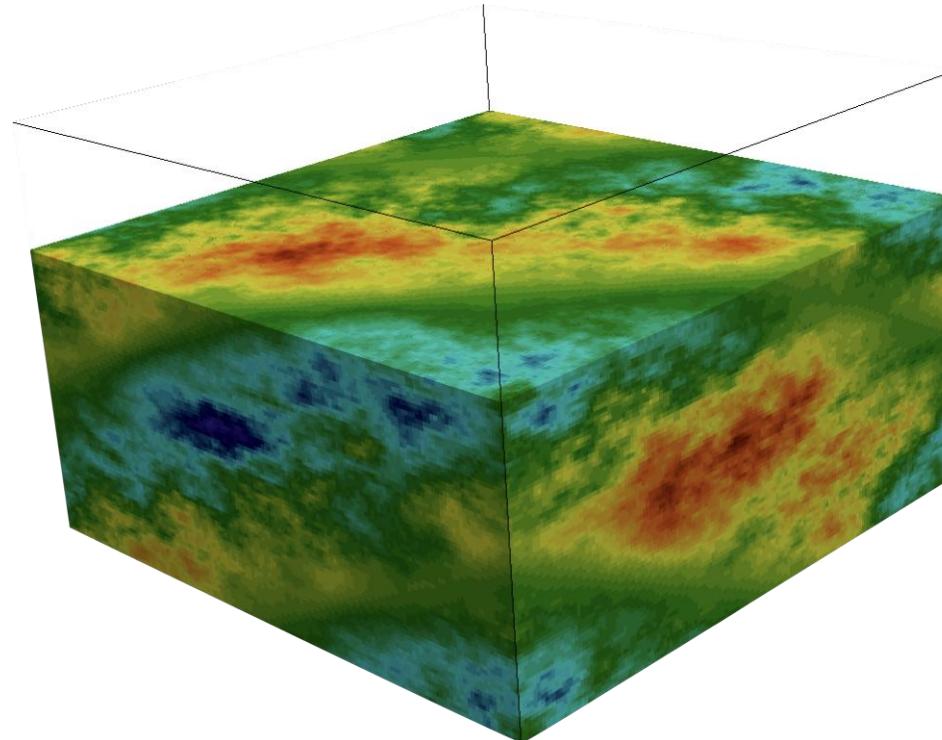
$$\bar{\sigma} = \begin{bmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{bmatrix}$$



# Automatic dielectric smoothing at Yee cell boundaries

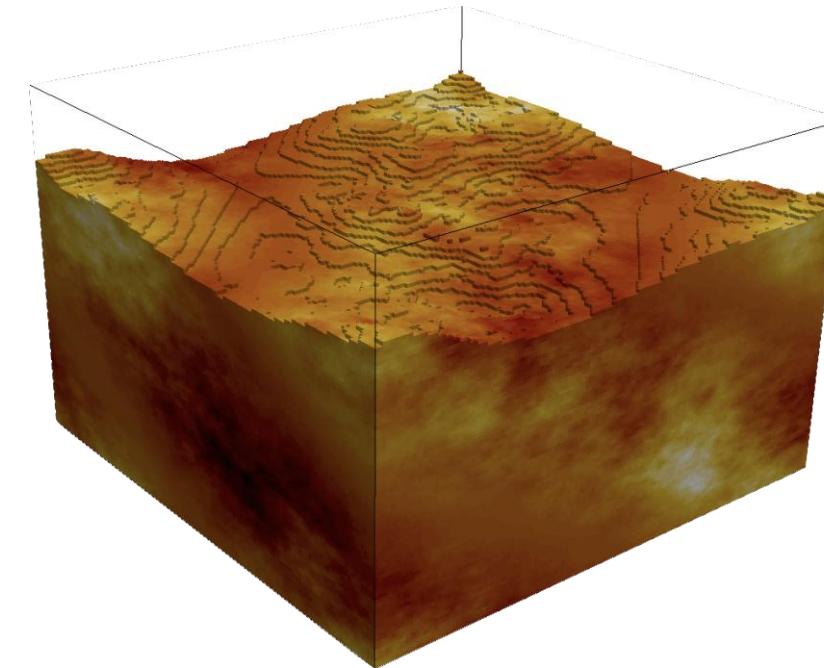
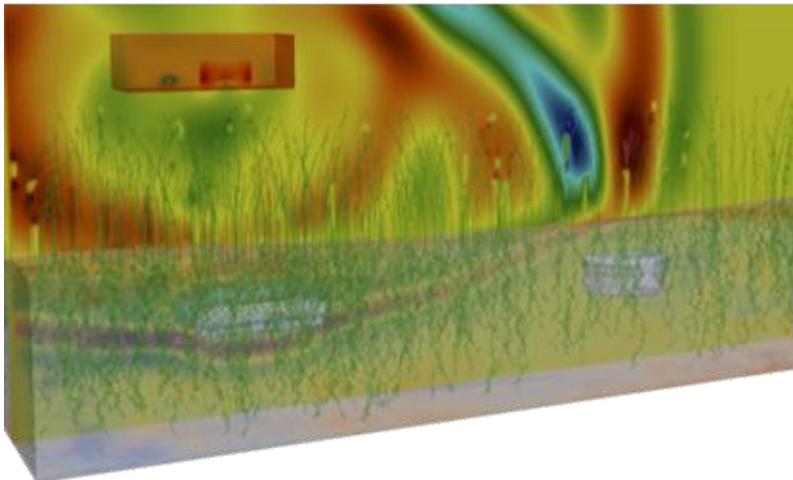
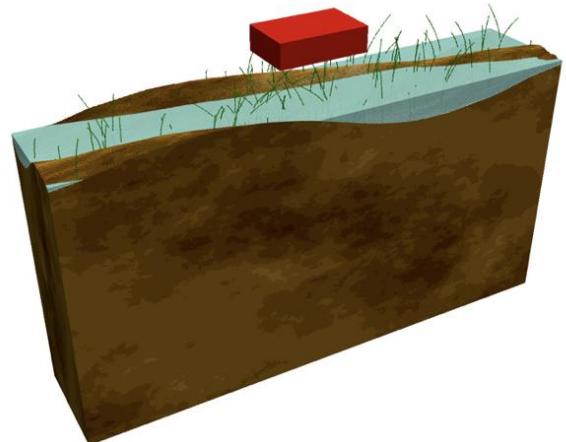


## **Soil or complex structure modelling: Stochastically distributed frequency depended properties of soils based on the Peplinski model**

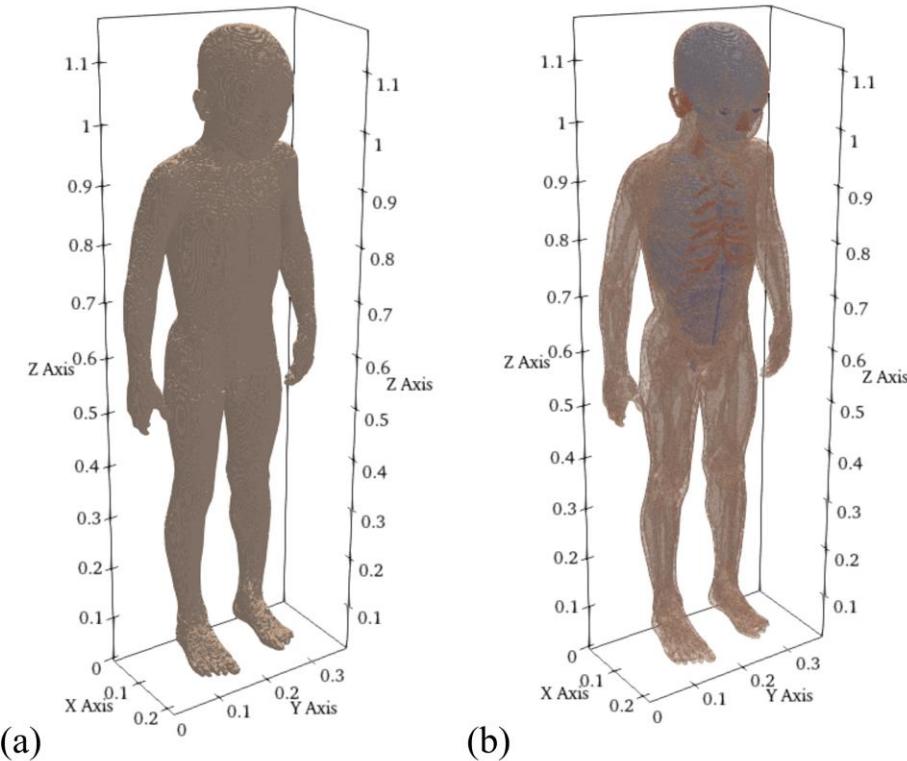
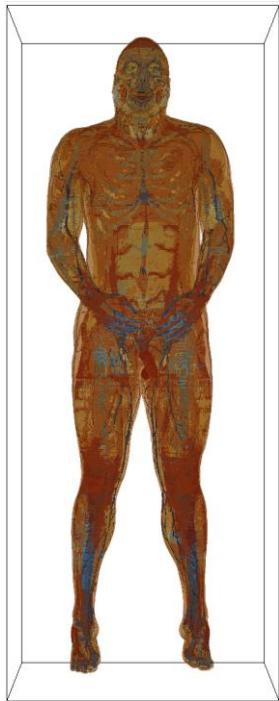


Giannakis, I., Giannopoulos, A., & Warren, C. (2016), "A Realistic FDTD Numerical Modeling Framework of Ground Penetrating Radar for Landmine Detection", *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, 9(1), 37-51

**Stochastic distribution of material properties, including rough surfaces, water puddles and even blades of grass!**



# Biomedical EM modelling



<https://itis.swiss/virtual-population/virtual-population/overview/>

<https://web.corral.tacc.utexas.edu/AustinManEMVoxels/AustinMan/index.html>

Massey, J., Geyik, C., Techachainiran, N., Hsu, C., Nguyen, R., Latson, T., Ball, M. & Yilmaz, A. (2012), "AustinMan and AustinWoman: High fidelity, reproducible, and open-source electromagnetic voxel models," in Proc. Bioelectromagnetics Soc. 34th Annual Meeting

# Simple example

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Please look up the detailed documentation where  
you can find examples!

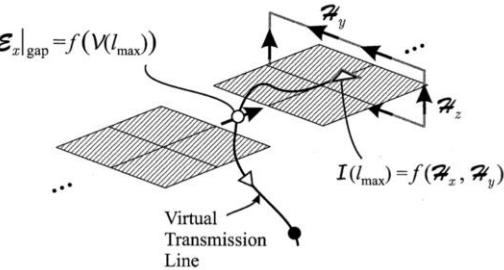
# Half-wavelength wire dipole antenna in free space

```
#title: Wire antenna - half-wavelength dipole in free-space
#domain: 0.050 0.050 0.200
#dx_dy_dz: 0.001 0.001 0.001
#time_window: 60e-9

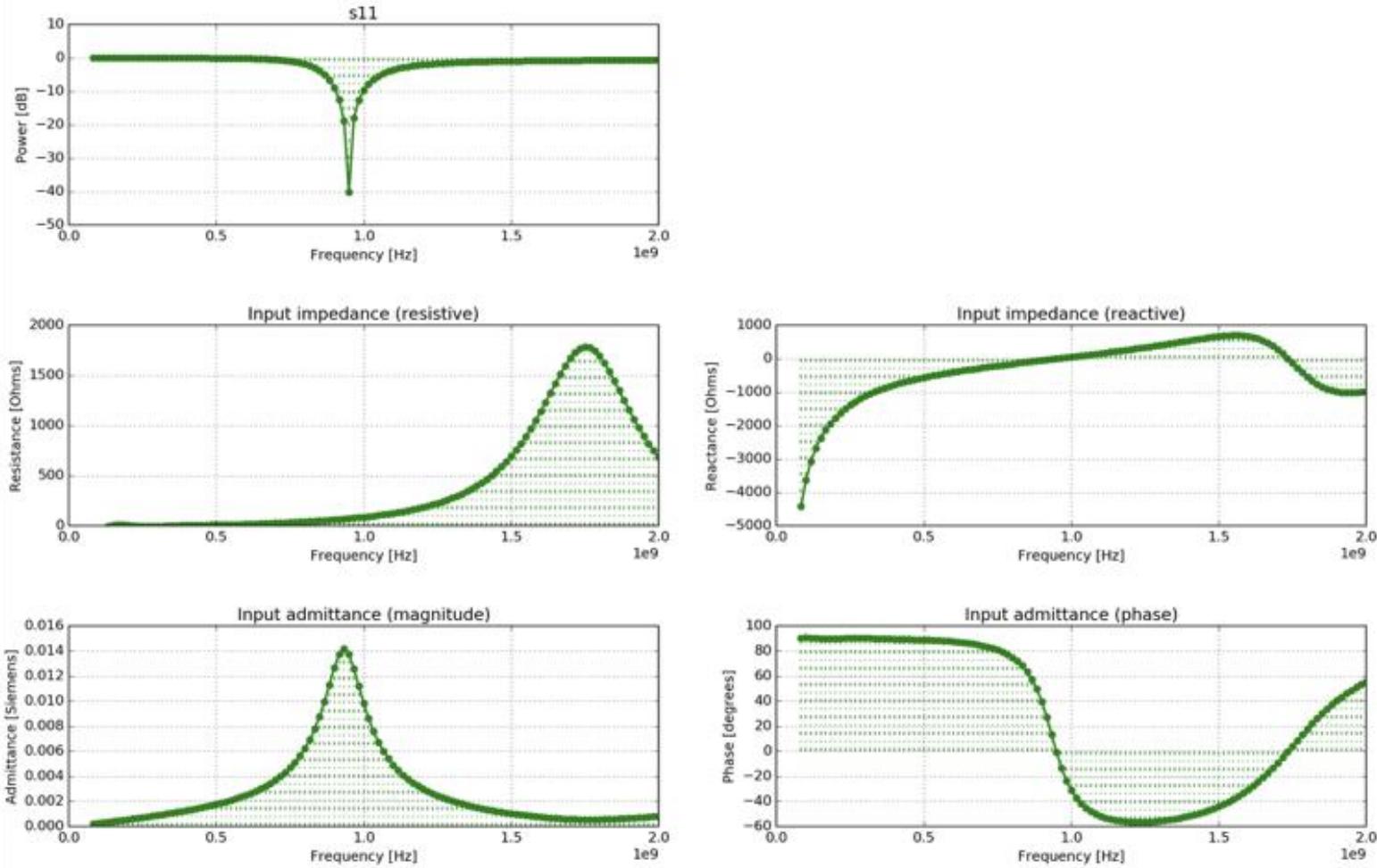
#waveform: gaussian 1 1e9 mypulse
#transmission_line: z 0.025 0.025 0.100 73 mypulse

## 150mm length
#edge: 0.025 0.025 0.025 0.025 0.025 0.175 pec
## 1mm gap at centre of dipole
#edge: 0.025 0.025 0.100 0.025 0.025 0.101 free_space
#geometry_view: 0.020 0.020 0.020 0.030 0.030 0.180 0.001 0.001 0.001 antenna_wire_dipole_fs f
```

Transmission-Line  
Feed:



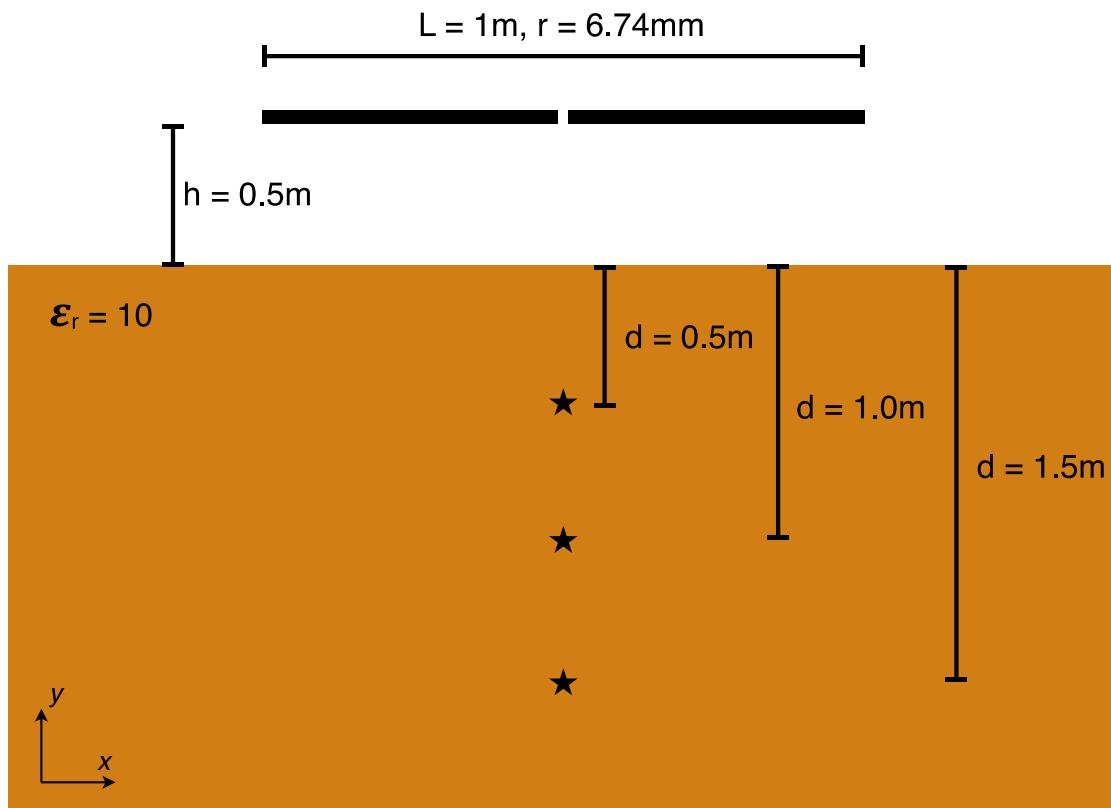
# Half-wavelength wire dipole antenna in free space



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the world

## Wire dipole antenna over a half-space



$$V(t) = V_0 e^{-g^2(t-t_0)^2},$$

$$V_0 = 1 \text{ V}$$

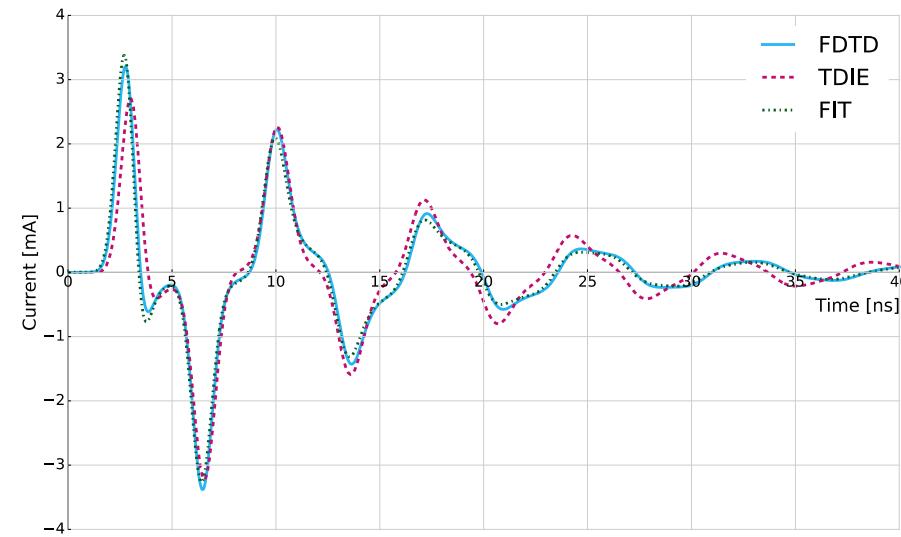
$$g = 1.5 \times 10^9$$

$$t_0 = 1.43 \times 10^{-9} \text{ s}$$

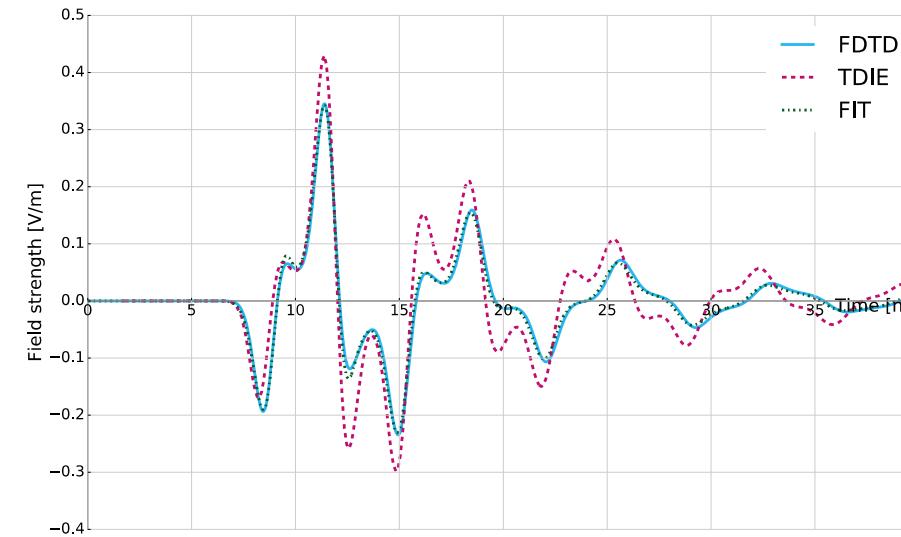
$$\Delta x = \Delta y = \Delta z = 10 \text{ mm}$$

$$f_c = 337 \text{ MHz}$$

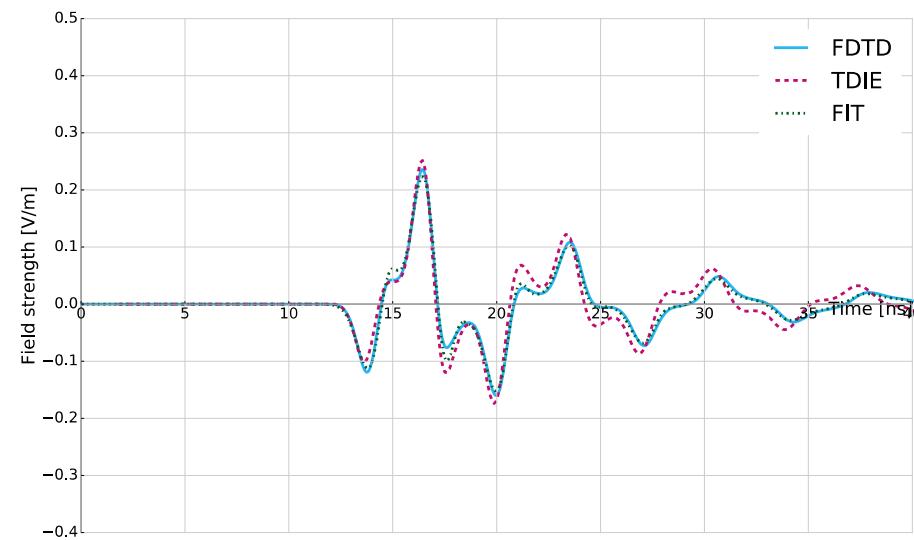
**I<sub>x</sub>@ feed**



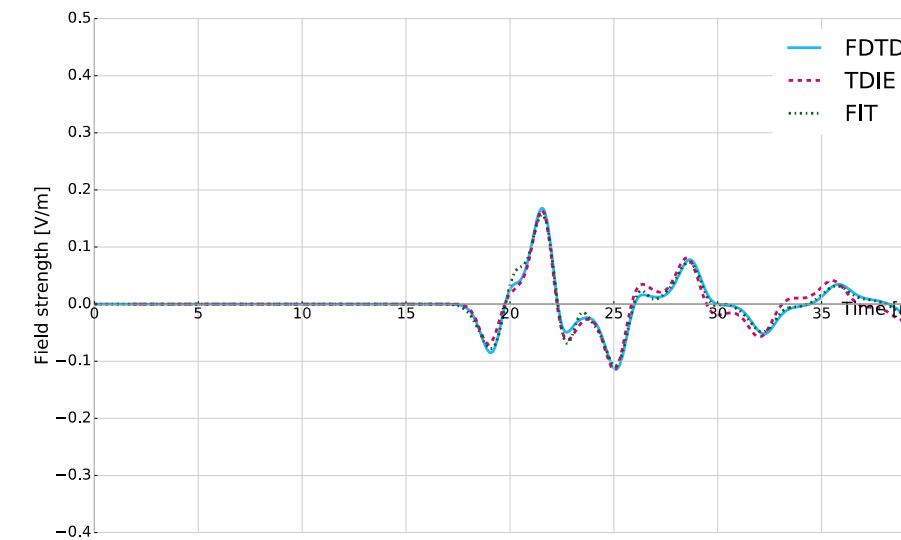
**Ex@ d=0.5m**



**Ex@ d=1.0m**



**Ex@ d=1.5m**

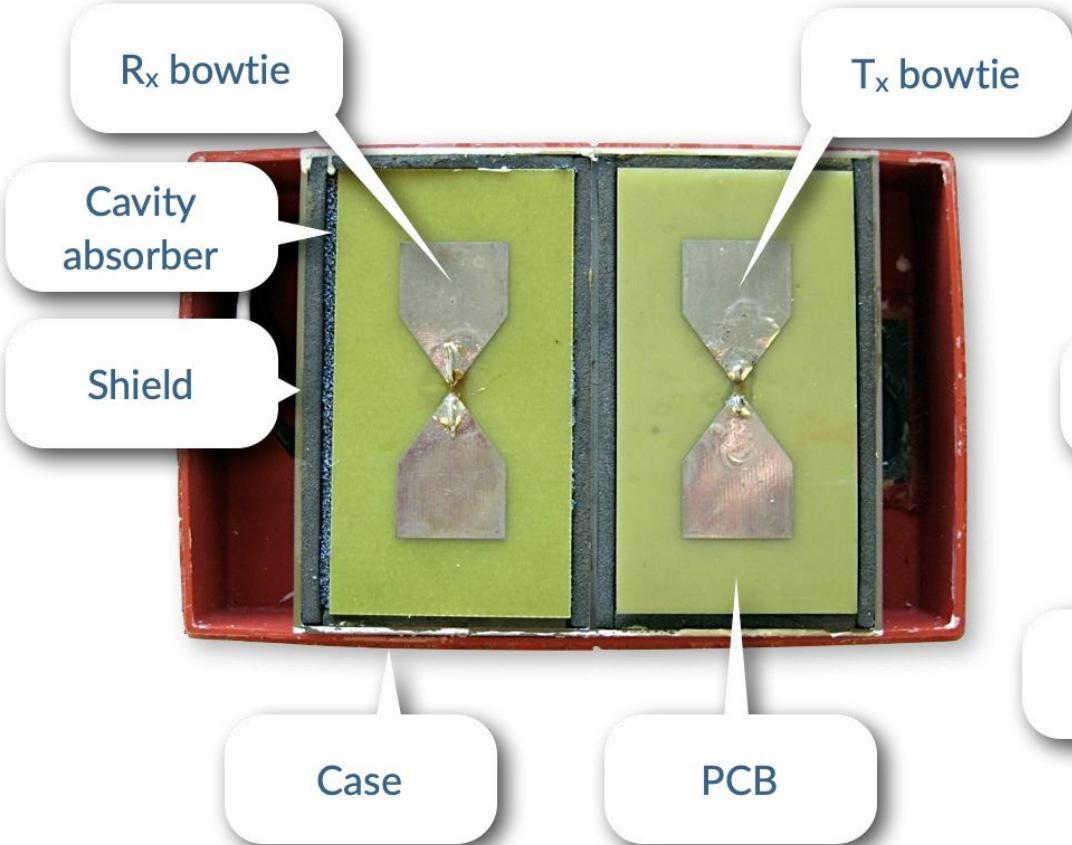


# Modelling GPR transducers

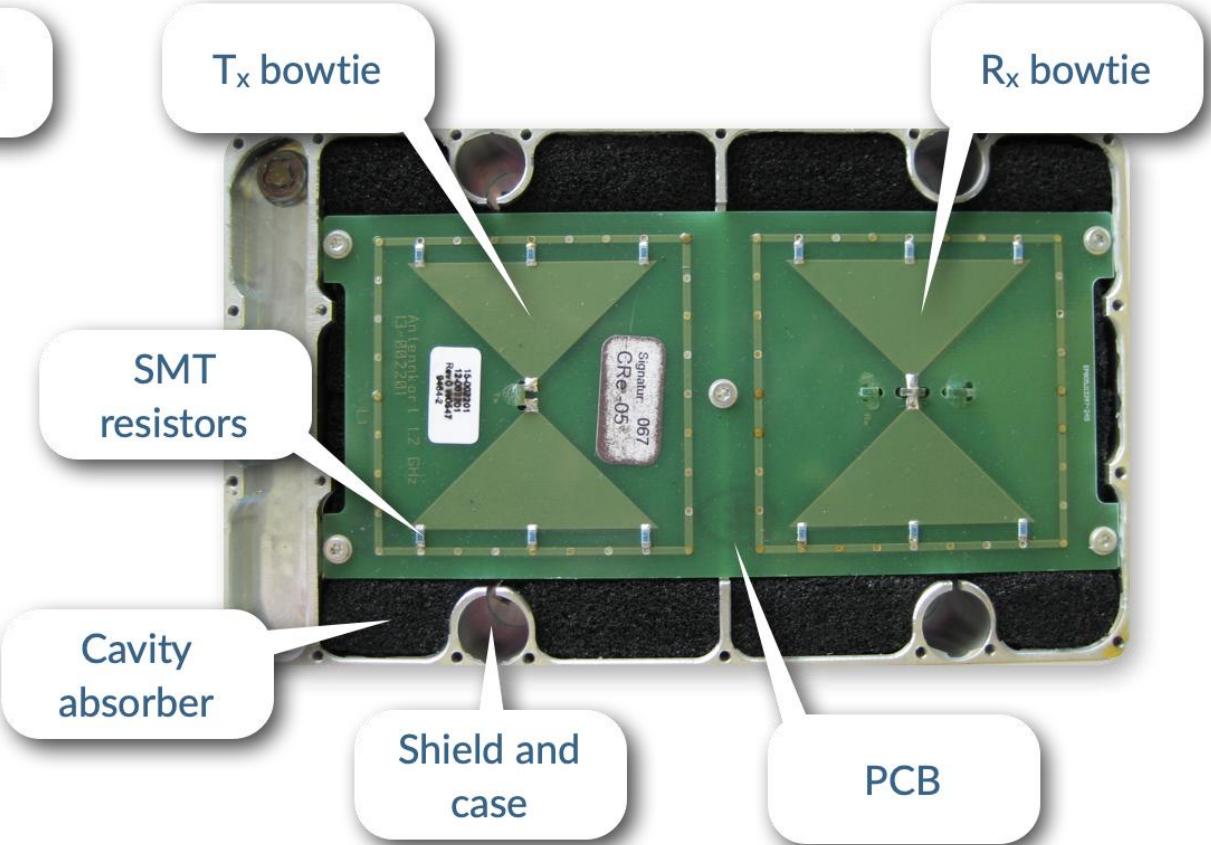
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# Commercial GPR antennas

GSSI 1.5GHz antenna

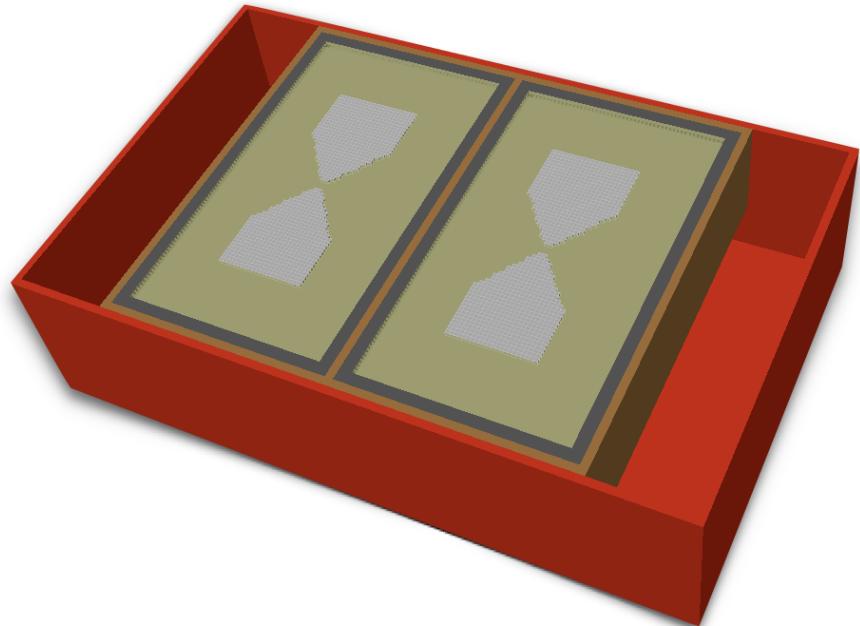


MALÅ 1.2GHz antenna

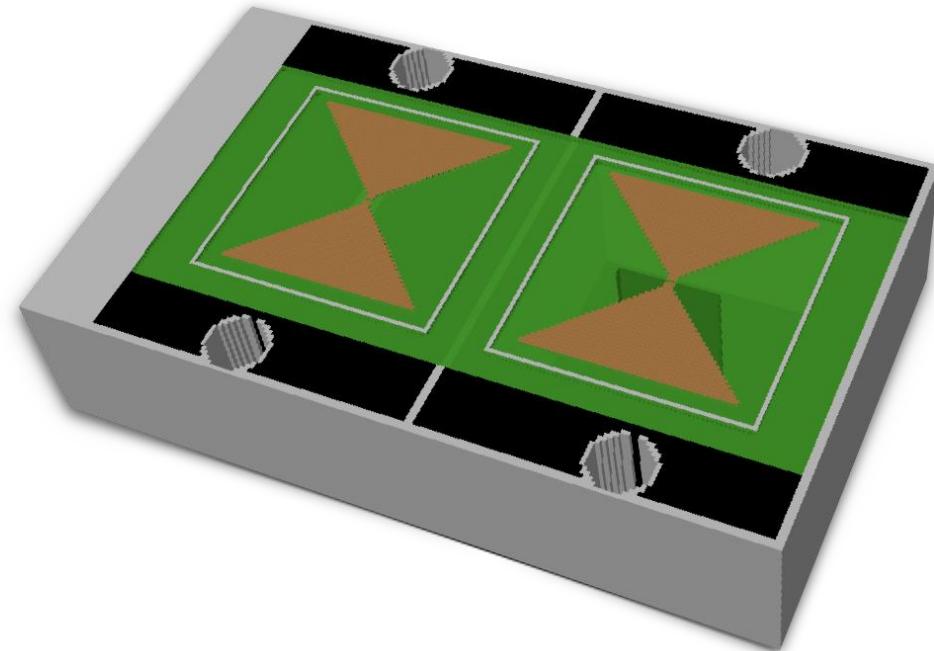


## FDTD antenna models of commercial GPR antennas

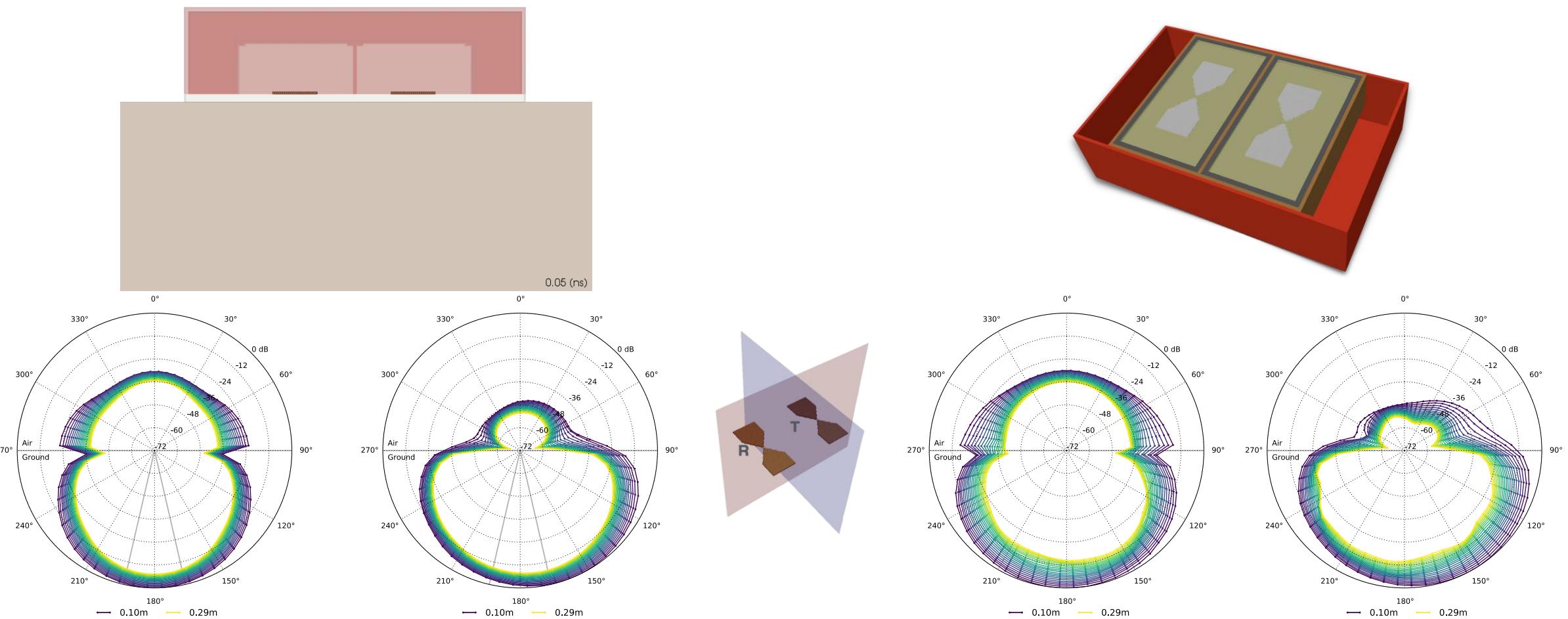
GSSI 1.5GHz antenna



MALA 1.2GHz antenna

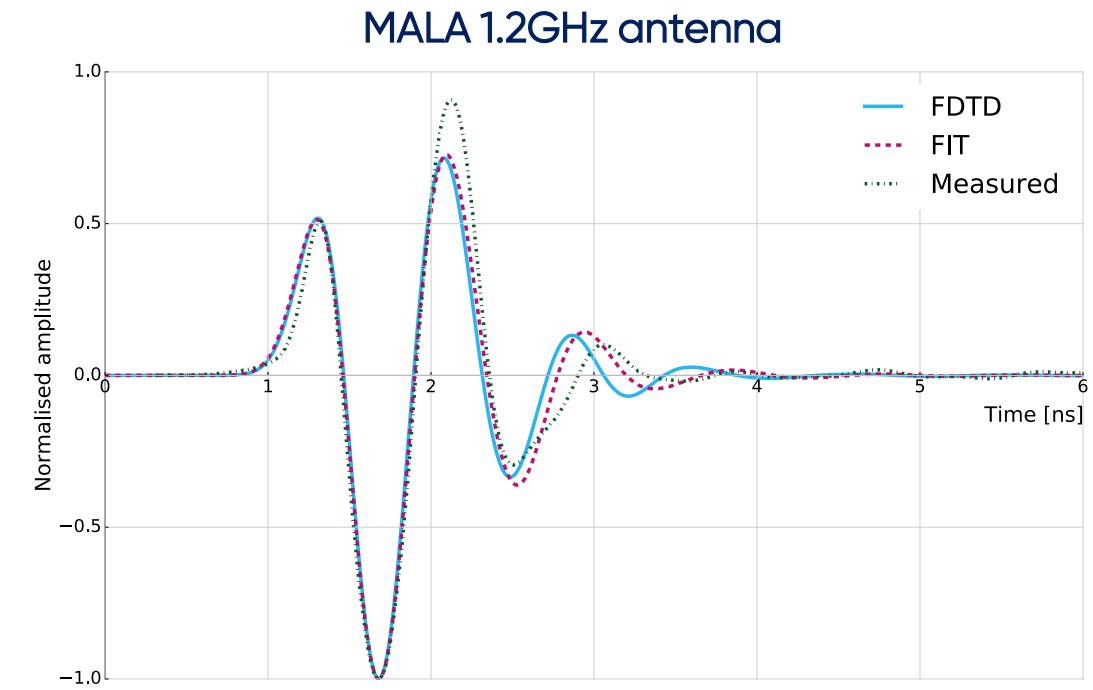
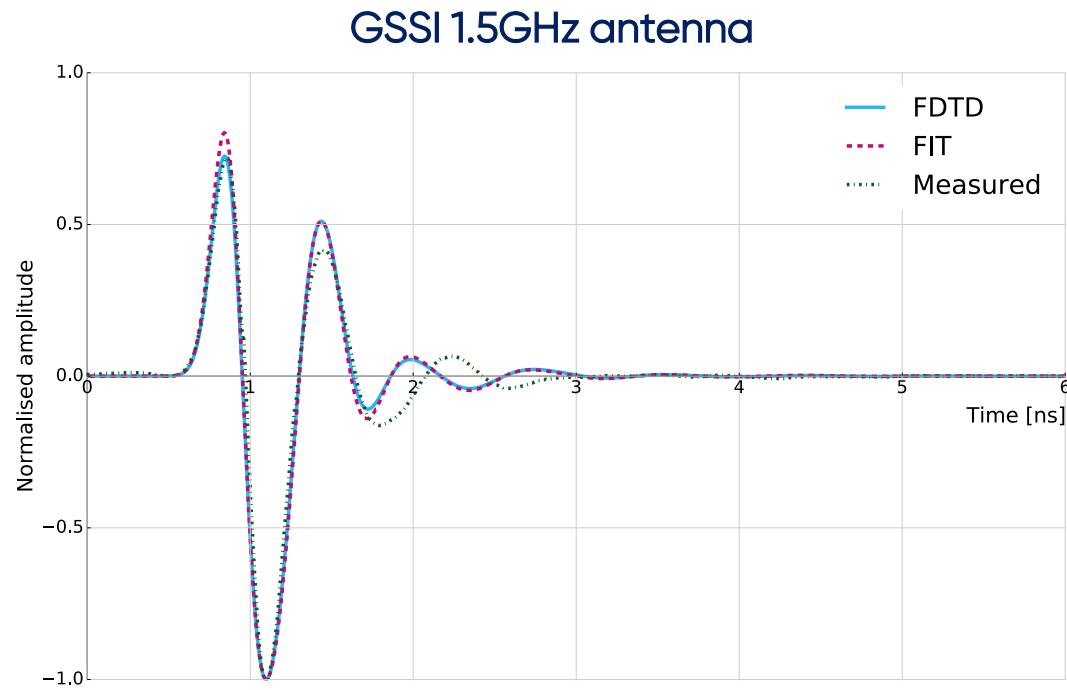


Warren, C. & Giannopoulos, A. (2011) Creating finite-difference time-domain models of commercial ground-penetrating radar antennas using Taguchi's optimization method, *Geophysics*, 76(2), G37-G47



Warren C. and Giannopoulos A., (2017) Characterisation of Ground Penetrating Radar antenna in Lossless Homogeneous and Lossy Heterogeneous Environments, Signal Processing, 132, pp. 221-226

# FDTD antenna models of commercial GPR antennas



# Advanced applications

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# GPR – Advanced data processing and Machine Learning



IEEE TRANSACTIONS ON GEOSCIENCE AND REMOTE SENSING, VOL. 61, 2023  
2003910

## GPR Full-Waveform Inversion With Deep-Learning Forward Modeling: A Case Study From Non-Destructive Testing

Ourania Patsia<sup>1</sup>, Antonios Giannopoulos<sup>1</sup>, and Iraklis Giannakis<sup>2</sup>

**Abstract**—Numerical modeling of ground penetrating radars (GPRs), such as the finite-difference time-domain (FDTD) method, has been extensively used to enhance the interpretation of GPR data and as a key component of full-waveform inversion (FWI). A major drawback of numerical solvers, especially within measures the slab thickness, and evaluates the condition and integrity of the concrete [2], [3], [4], [5]. In particular, when it comes to locating the reinforcement in concrete structures, GPR is very effective due to the high contrast between the

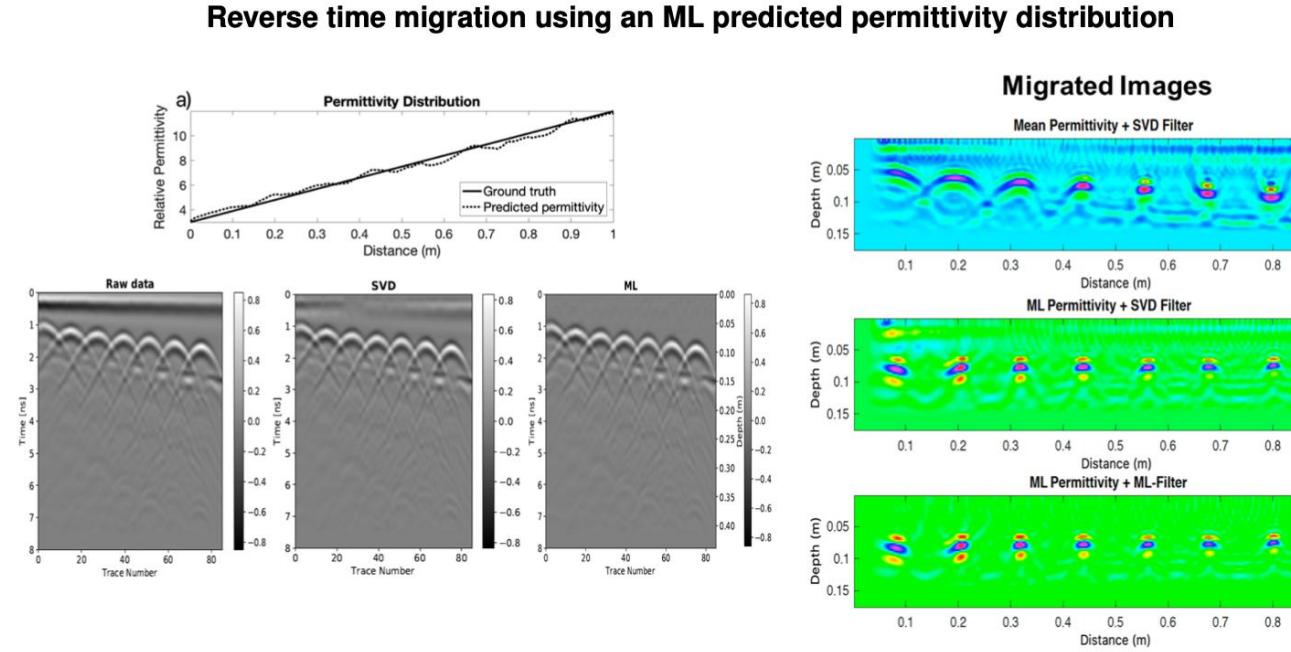
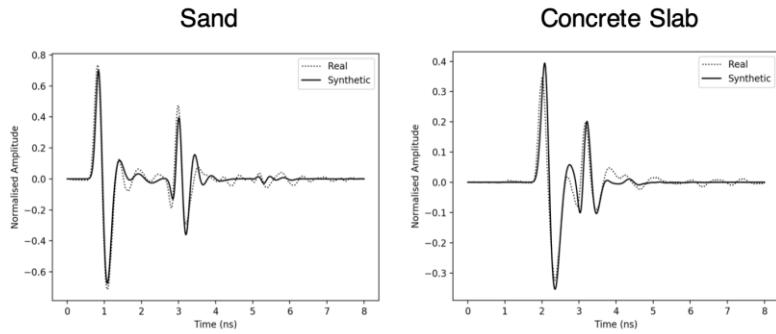
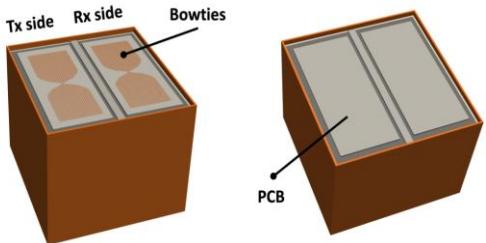
IEEE TRANSACTIONS ON GEOSCIENCE AND REMOTE SENSING, VOL. 61, 2023  
2003311

## Background Removal, Velocity Estimation, and Reverse-Time Migration: A Complete GPR Processing Pipeline Based on Machine Learning

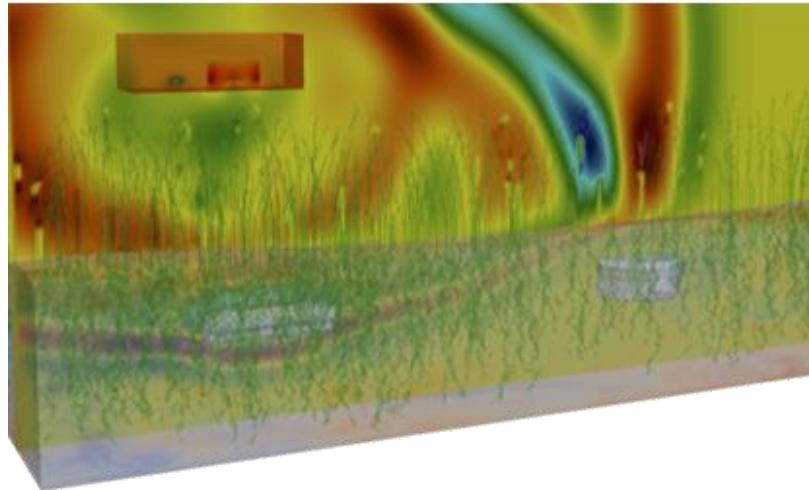
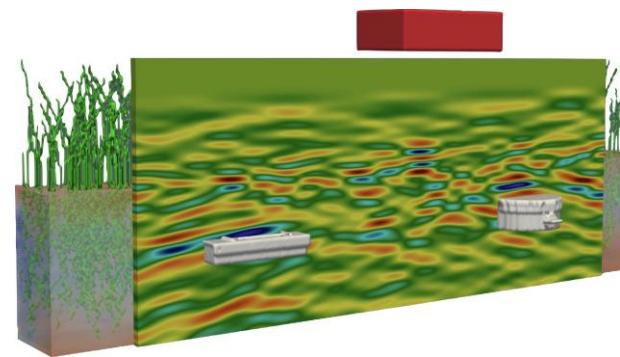
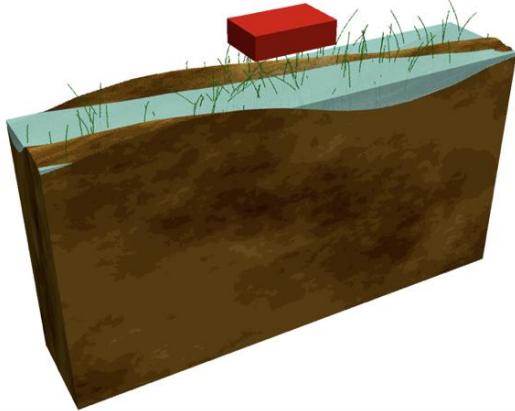
Ourania Patsia<sup>1</sup>, Antonios Giannopoulos<sup>1</sup>, and Iraklis Giannakis<sup>2</sup>

**Abstract**—The performance of ground-penetrating radar (GPR) is greatly influenced by the cross coupling between the transmitter and the receiver, and the response from the background. Their combined effect often masks the weaker target signals, especially in cases where shallow buried targets are present. Moreover, errors in velocity estimation result to over/under-migrated images, which further compromises the

Regardless of the application, the GPR signals are often masked by the direct air and ground wave response. This is known as background clutter and is typically subtracted from the total response. Subsequently, the velocity of the medium is evaluated, typically done via hyperbola fitting. Finally, the velocity of the medium is used as an input in migration,



# GPR - Landmines



IEEE JOURNAL OF SELECTED TOPICS IN APPLIED EARTH OBSERVATIONS AND REMOTE SENSING, VOL. 9, NO. 1, JANUARY 2016

37

## A Realistic FDTD Numerical Modeling Framework of Ground Penetrating Radar for Landmine Detection

Iraklis Giannakis, Antonios Giannopoulos, and Craig Warren

**Abstract**—A three-dimensional (3-D) finite-difference time-domain (FDTD) algorithm is used in order to simulate ground penetrating radar (GPR) for landmine detection. Two bowtie GPR transducers are chosen for the simulations and two widely employed antipersonnel (AP) landmines, namely PMA-1 and PMN are used. The validity of the modeled antennas and landmines is tested through a comparison between numerical and laboratory measurements. The modeled AP landmines are buried in a realistically simulated soil. The geometrical characteristics of soil's inhomogeneity are modeled using fractal correlated noise, which gives rise to Gaussian semivariograms often encountered in the field. Fractals are also employed in order to simulate the

A better understanding of the scattering mechanisms within the ground can help us increase the effectiveness of GPR and investigate its limitations. This can be achieved through numerical modeling that can provide insight on how the soil's characteristics can influence the overall performance of GPR. Apart from that, numerical modeling can be a practical tool for testing and comparing different antennas and processing algorithms in a wide range of environments. Furthermore, a realistic numerical model can also be employed for training purposes in machine learning based approaches. In order to address

# GPR – Planetary

2484

IEEE JOURNAL OF SELECTED TOPICS IN APPLIED EARTH OBSERVATIONS AND REMOTE SENSING, VOL. 14, 2021

## Ground-Penetrating Radar Modeling Across the Jezero Crater Floor

Sigurd Eide<sup>1</sup>, Svein-Erik Hamran, Henning Dypvik, and Hans E. F. Amundsen

**Abstract**—This article assesses how the ground-penetrating radar REMFAX will image the crater floor at the Mars 2020 landing site, where lithological compositions and stratigraphic relationships are under discussion prior to mission operation. A putative mafic unit (lava flow) has been identified and defined on the crater floor with a crucial role in piecing together the chronology of deposition and for understanding the volcanic history in the region. In order to see how lithological properties affect radar sounding, a synthetic radargram is generated through numerical modeling using finite-difference time-domain method. The acquisition is simulated across the mafic unit as a succession of lava flows, exploring detection of internal structures and contacts to adjacent lithologies. To compare modeling results with the alternative formation scenarios, a discussion about sounding over a ferromagnetic material is presented. Similarities and differences between Martian and terrestrial lithologies can be related to electromagnetic properties relevant for radar sounding. This article, therefore, evaluates potential scientific insights gained from acquisition across the disputed mafic unit, in light of proposed hypotheses of lithological generation.

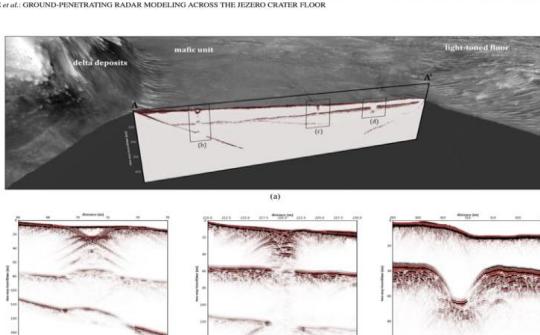


Fig. 4. (a) Synthetic radargram displays the results from modeling radar sounding over the 400 m acquisition traverse (A-A'). Note that the radargram is aligned with the topography, but its vertical axis below the surface is in two-way travel time [ns] and has a vertical exaggeration of  $\times 2.0$ , assuming a constant medium velocity of 0.12 m/ns. Image zooms in (b) on the impact crater, (c) on the vertical fracture, and (d) on the subsurface crater structure.

Hindawi  
International Journal of Antennas and Propagation  
Volume 2017, Article ID 3013249, 11 pages  
<https://doi.org/10.1155/2017/3013249>



## Research Article

### Numerical Simulations of the Lunar Penetrating Radar and Investigations of the Geological Structures of the Lunar Regolith Layer at the Chang'E 3 Landing Site

Chunyu Ding,<sup>1,2,3</sup> Yan Su,<sup>1,2</sup> Shuguang Xing,<sup>1,2</sup> Shun Dai,<sup>1,2</sup> Yuan Xiao,<sup>1,2,3</sup> Jianqing Feng,<sup>1,2</sup> Danqing Liu,<sup>4</sup> and Chunhai Li<sup>1,2</sup>

<sup>1</sup> Key Laboratory of Lunar and Deep Space Exploration, Chinese Academy of Sciences, Beijing 100012, China

<sup>2</sup> National Astronomical Observatory, Chinese Academy of Sciences, Beijing 100012, China

<sup>3</sup> University of Chinese Academy of Sciences, Beijing 100049, China

<sup>4</sup> Renmin University of China, Beijing 100872, China

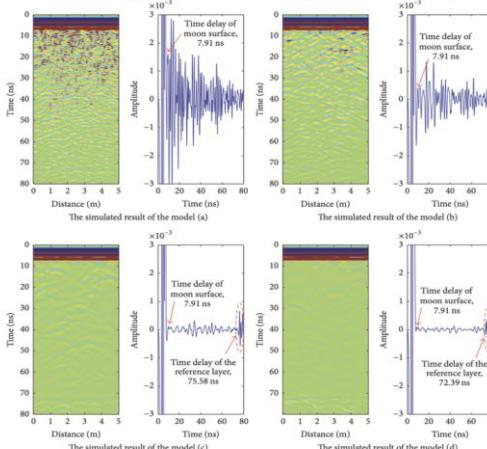
Correspondence should be addressed to Yan Su; [suyan@nao.cas.cn](mailto:suyan@nao.cas.cn)

Received 21 December 2016; Revised 12 March 2017; Accepted 3 April 2017; Published 23 May 2017

Academic Editor: Han Guo

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In the process of lunar exploration, and specifically when studying lunar surface structure and thickness, the established lunar regolith model is usually a uniform and ideal structural model, which is not well-suited to describe the real structure of the lunar regolith layer. The present study aims to explain the geological structural information contained in the channel 2 LPR (lunar penetrating radar) data. In this paper, the random medium theory and Apollo drilling core data are used to construct a



Icarus 408 (2024) 115837

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## Research Paper

### Evidence of shallow basaltic lava layers in Von Kármán crater from Yutu-2 Lunar Penetrating Radar

Iraklis Giannakis<sup>a,\*</sup>, Javier Martin-Torres<sup>a</sup>, Yan Su<sup>b</sup>, Jianqing Feng<sup>c</sup>, Feng Zhou<sup>d</sup>, Maria-Paz Zorzano<sup>e</sup>, Craig Warren<sup>f</sup>, Antonios Giannopoulos<sup>g</sup>

<sup>a</sup> University of Aberdeen, School of Geosciences, Aberdeen, UK

<sup>b</sup> National Astronomical Observatories, Chinese Academy of Sciences, China

<sup>c</sup> University of Chinese Academy of Sciences, Beijing 100049, China

<sup>d</sup> Remin University of China, Beijing 100872, China

<sup>e</sup> Centro de Astrobiología (CAB), CSIC-INTA, Torrejón de Ardoz, Madrid, Spain

<sup>f</sup> Northumbria University, Northumbria, UK

<sup>g</sup> The University of Edinburgh, Edinburgh, UK

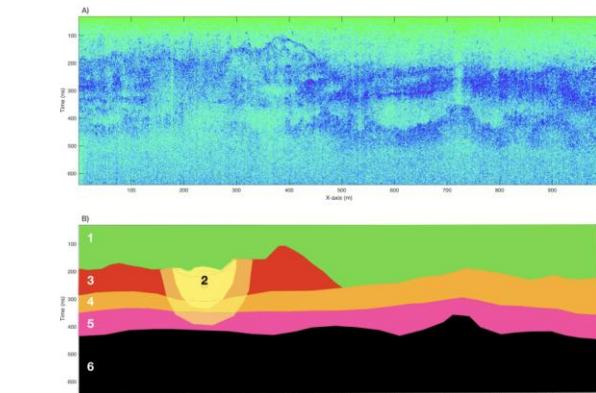
## ARTICLE INFO

Keywords:  
Chang'E-4

## ABSTRACT

Yutu-2 – the rover from the Chang'E-4 mission – is the longest operational Lunar rover, and the first rover to land on the far side of the Moon. It is the second planetary rover to be equipped with ground-penetrating

I. Giannakis et al.



Icarus 408 (2024) 115837

| epcc |

# Now and the future of gprMax

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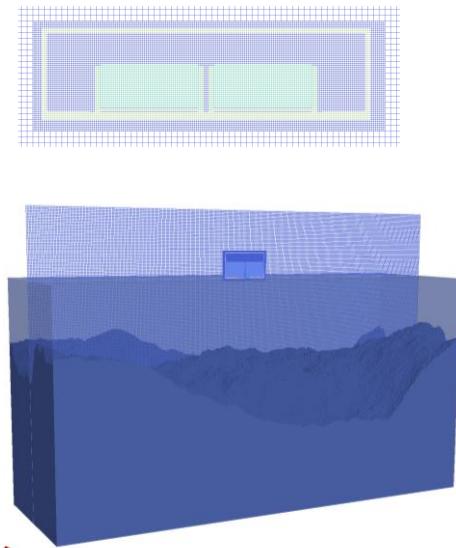
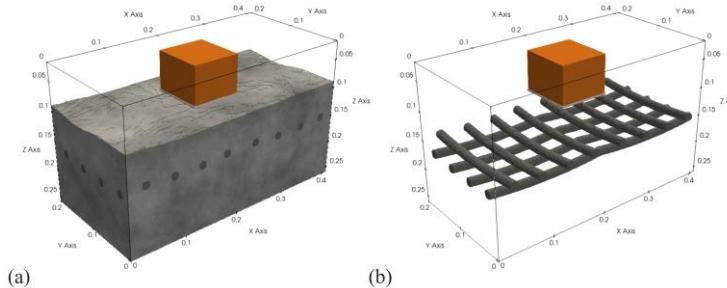
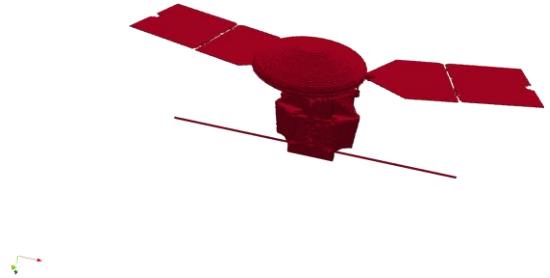


Google  
Summer of Code

We participated in  
GSoC in 2019, 2021,  
2023, 2024 and in 2025

Google Summer of Code

 <p><b>LIBRE CUBE</b> open source space exploration</p> <p>LibreCube Initiative Open Source Space Exploration</p>	 <p><b>Open</b> Chemistry</p> <p>Open Chemistry Advancing Open Source &amp; Open Science for Chemistry</p>	 <p><b>CGAL Project</b> C++ library of computational geometry</p>
 <p><b>SageMath</b> Open-source mathematics software system</p>	 <p><b>INCF</b> An open &amp; FAIR neuroscience standards organization</p>	 <p><b>GNSS-SDR</b> An open source GNSS software-defined receiver</p>
 <p><b>caMicroscope</b> Toolkit for cancer imaging research</p>	 <p><b>gprMax</b> Simulating electromagnetic wave propagation</p>	 <p><b>GNU Radio</b> The free &amp; open software radio ecosystem</p>
 <p><b>DeepChem</b> Democratize AI for drug discovery.</p>	 <p><b>python™</b> Python Software Foundation A programming language used for science &amp; more</p>	 <p><b>GNU Octave</b> Free Your Numbers</p>



## Next version of gprMax - beta testing 18-Jul-2023



We are almost ready to release the next version of gprMax (v4) code named Carn Mor, continuing our single malt Scotch whisky theming! Carn Mor has a number of new and exciting features such as:

- **Sub-gridding** - the ability to define different spatial resolutions in different areas of the main grid. This allows high-dielectric materials and fine geometries to be more efficiently modelled.
- **OpenCL support** - run your simulations more quickly on hardware (CPU and GPU) that supports OpenCL.
- **STLtoVoxel toolbox** - convert STL files and import complex geometries without having to build them from geometry commands.
- **DebyeFit toolbox** - simulate materials with dispersive properties described by relaxation models such as Havriliak-Negami, Jonscher, Complex Refractive Index Mixing (CRIM), or your own measured data.
- **Landmine toolbox** - contains realistic models of anti-personnel (AP) landmines including the PMA-1, PMN, and TS-50.

There are many more new features and also lots of under-the-hood improvements. We are seeking current gprMax users to beta test this new version which is available through the [devel branch on our GitHub repository](#). Please report bugs through our [GitHub issue tracker](#) and use the tag `v4 bug`.

# eCSE project:

---



*Large-scale open-source computational electrodynamics:  
MPI domain decomposition for gprMax*

# Why MPI domain decomposition?

- Maximum model size on a single node of ARCHER2 (256GB memory):
  - 1.6m x 1.6m x 1.6m model at 1mm resolution
  - $4.096\text{m}^3$  or  $4.096 \times 10^9$  cells
- Using more complex geometry increases memory usage
- Taking snapshots can increase memory usage

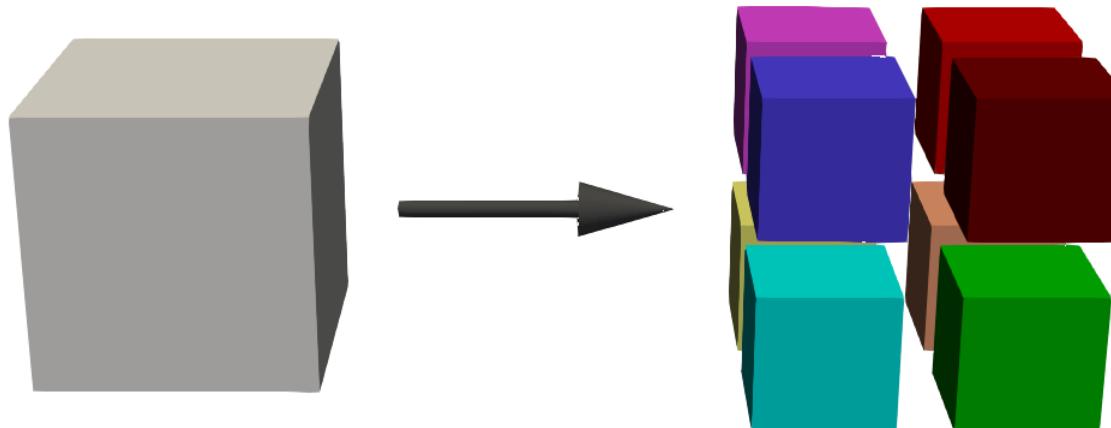
# Why MPI domain decomposition?

- Existing gprMax solvers:
  - CPU (OpenMP)
  - GPU (CUDA)
  - OpenCL
- All of these solvers are limited to a single node or device
- To run larger simulations, we need more memory
- HPC systems do have nodes with large amounts of memory, but:
  - Limit to OpenMP scaling within a node
  - MPI scales beyond a single node (and hopefully adds performance too)

# Adding MPI domain decomposition

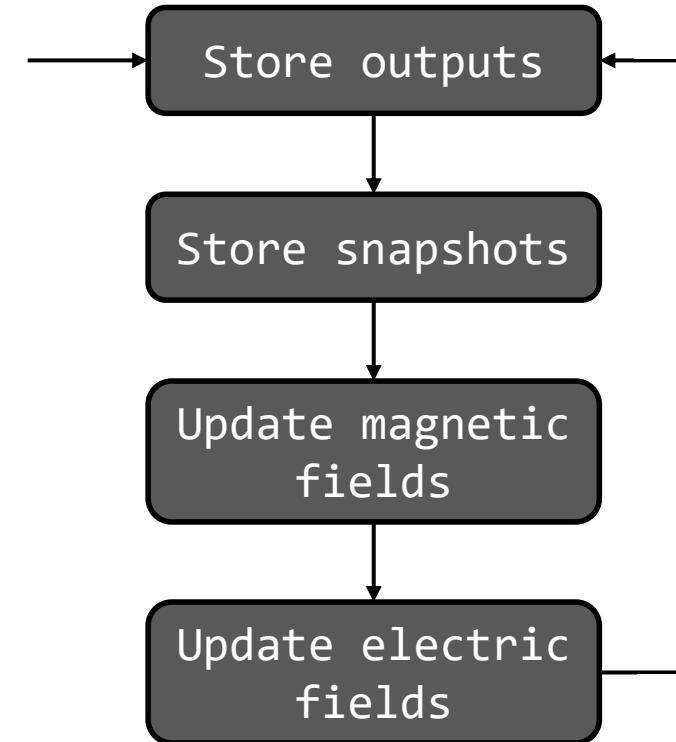
- Minimal changes for users – no need to change the model definition
- Control decomposition using the new `--mpi` flag

```
$ mpirun -n 8 python -m gprMax model.in --mpi 2 2 2
```



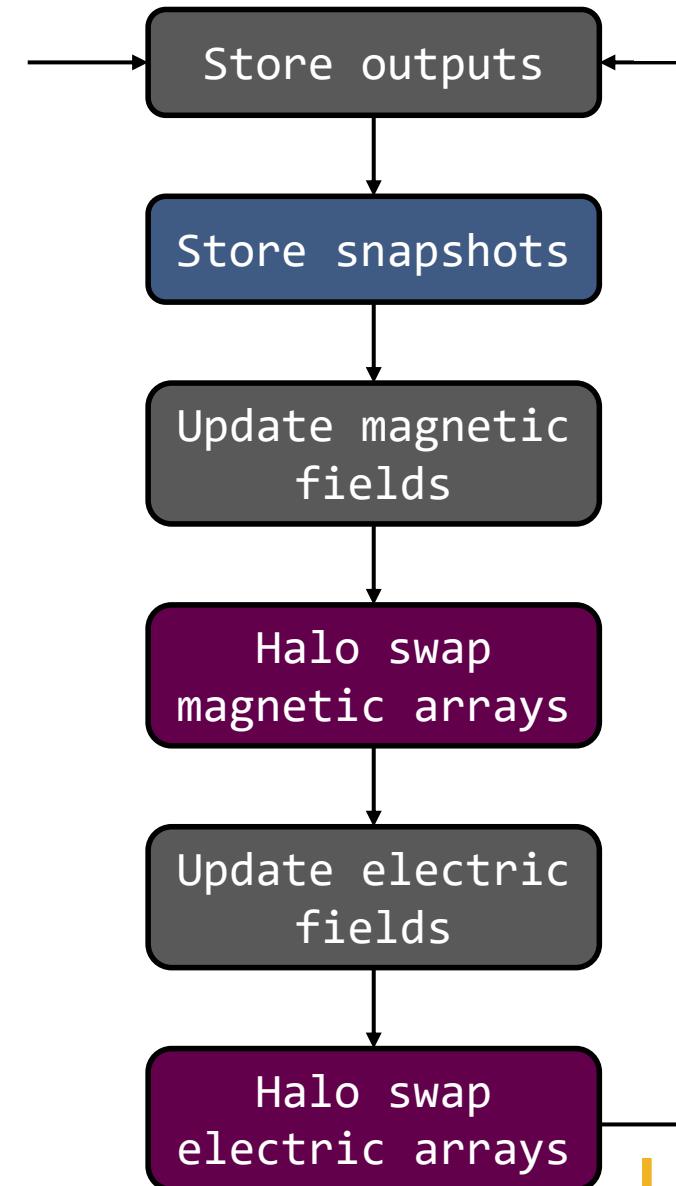
# Solver Loop

- Simplified control flow of the main solver



# Solver Loop

- Simplified control flow of the main solver
- Addition of halo exchanges
  - Direct point to point communication with neighbours
  - Asynchronous communication
- Store snapshots
  - Snapshot resolution may be lower than the main grid
  - Each snapshot requires own halo exchange
  - No actual I/O, so no collective communication



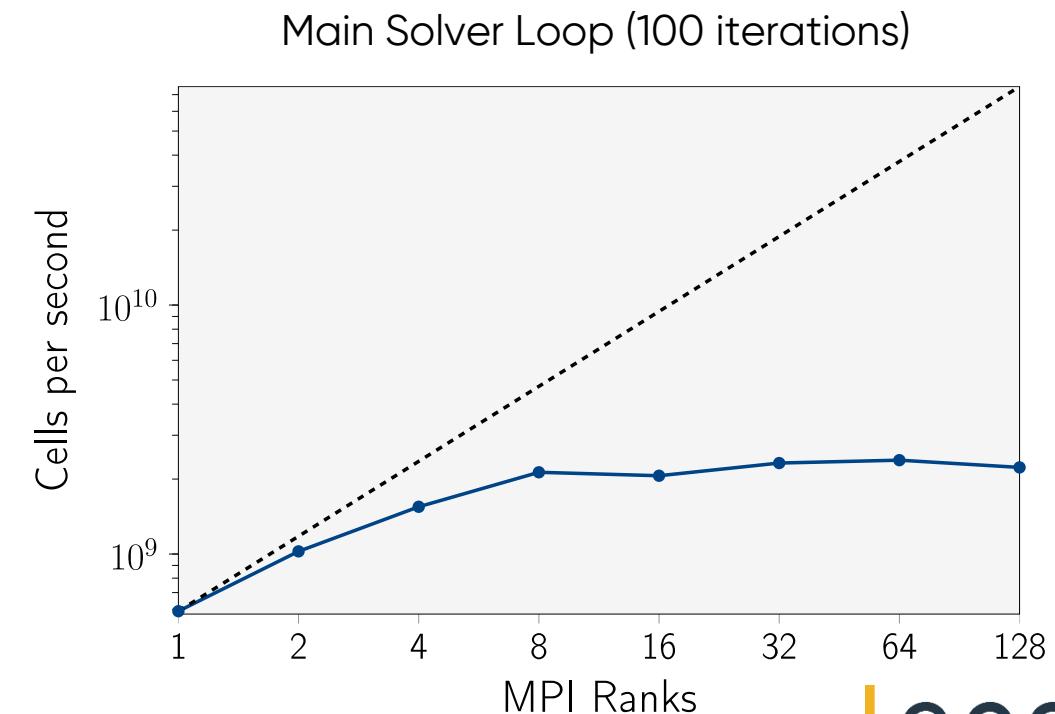
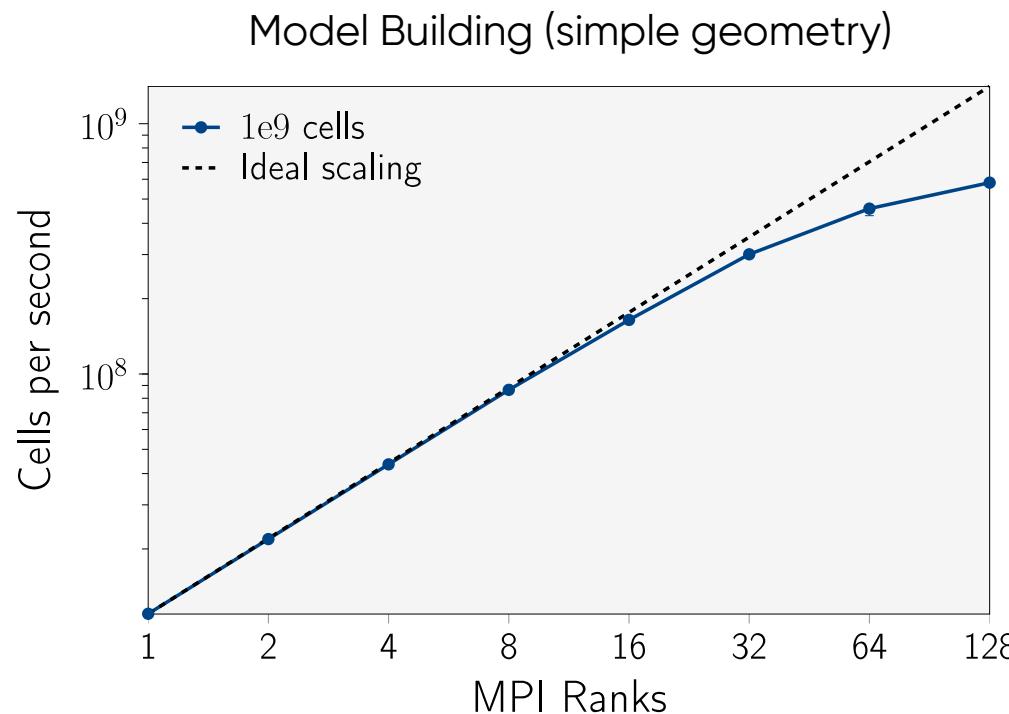
# Model Building

- Ranks build their own local grid
- No OpenMP parallelisation for this part of the code
  - Lots of room for improvement with MPI
- Result is insensitive to the domain decomposition
- Ranks map from the global coordinate space to the local coordinate space
- Fractal objects and I/O objects were the biggest challenge

# Single Node Performance

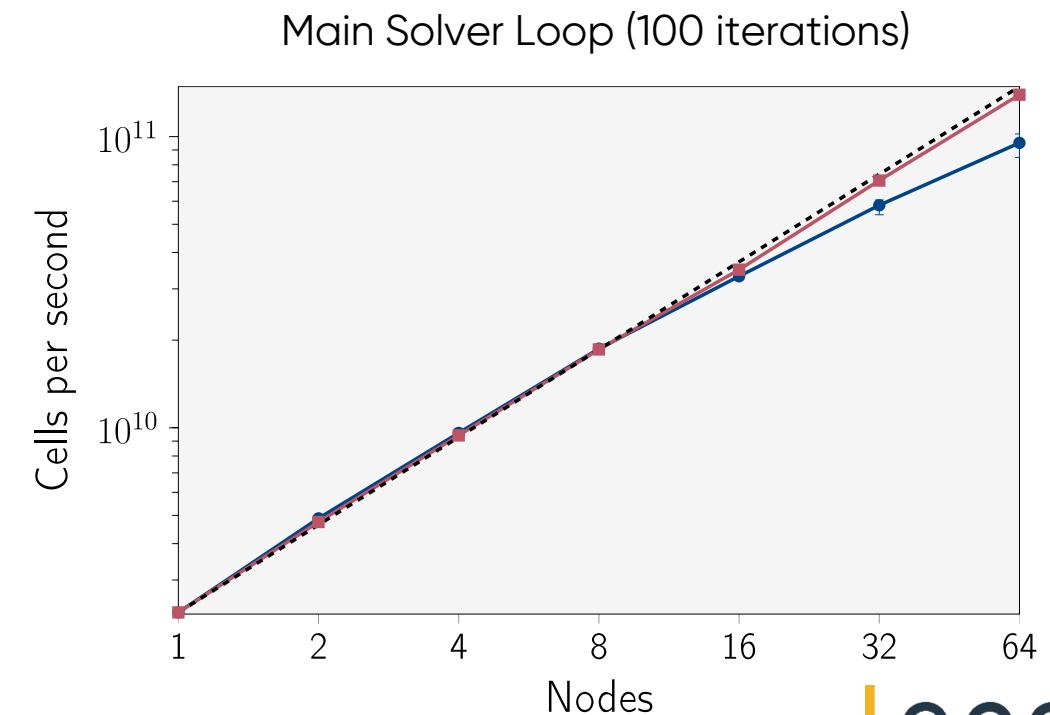
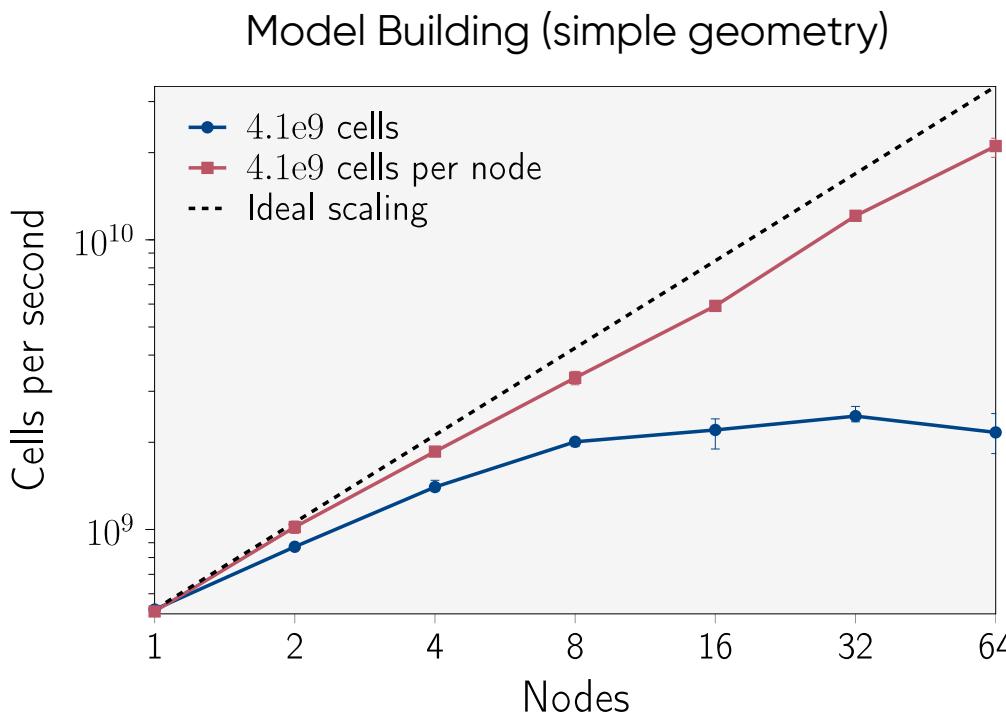
- Simulation uses ~ 53.2 GB of memory
- The node is fully populated throughout

1 MPI rank → 128 OpenMP threads per rank  
8 MPI ranks → 16 OpenMP threads per rank  
Etc...



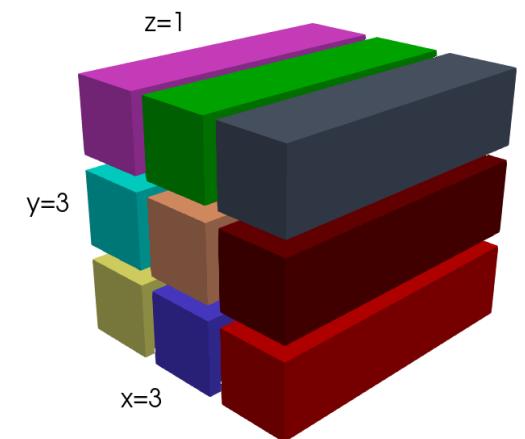
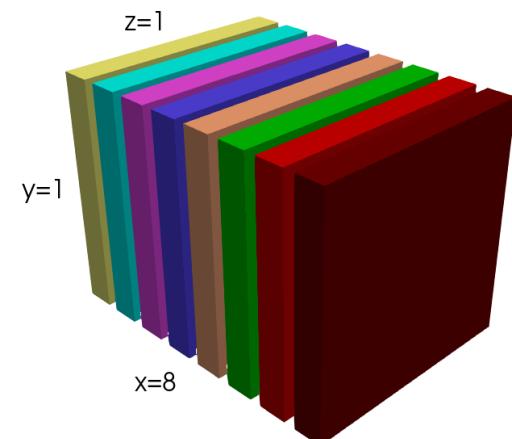
# Multi Node Performance

- Chose the best performing single-node configuration:
  - 64 MPI ranks per node and 2 OpenMP threads per rank
- Largest model:  $2.6 \times 10^{11}$  cells,  $\sim 14.4$  TB of memory across 64 nodes



# Model Building – Fractal Geometry

- Used for stochastic materials (e.g. soil models) and surface roughness
- Perform an FFT over a 2D or 3D array of random numbers
- Limits domain decomposition – must be 1 in at least one dimension
  - 1D (slab) or 2D (pencil) – not 3D
- Choice of decomposition can dramatically effect performance
- Needs to be reproducible in parallel



# Model Building – Fractal Geometry

- Initial attempt ~100 times slower than serial baseline
  - Iterate over global grid and generate random numbers one at a time
  - Keep if within the local grid. Otherwise discard
- Instead calculate blocks of random numbers to either keep or discard

Implementation	MPI Ranks	OpenMP Threads	Time in generate_fractal_volume()	Percentage of total runtime in generate_fractal_volume()
Serial	-	32	34.4s	2.9%
Original MPI	8	16	3135.7s	82.7%
Updated MPI	8	16	24.2s	3.5%

**Note:** The MPI runs used `--mpi 1 2 4` as the decomposition. It is likely `--mpi 1 1 8` would improve the overall performance further.

# VTKHDF for Parallel I/O

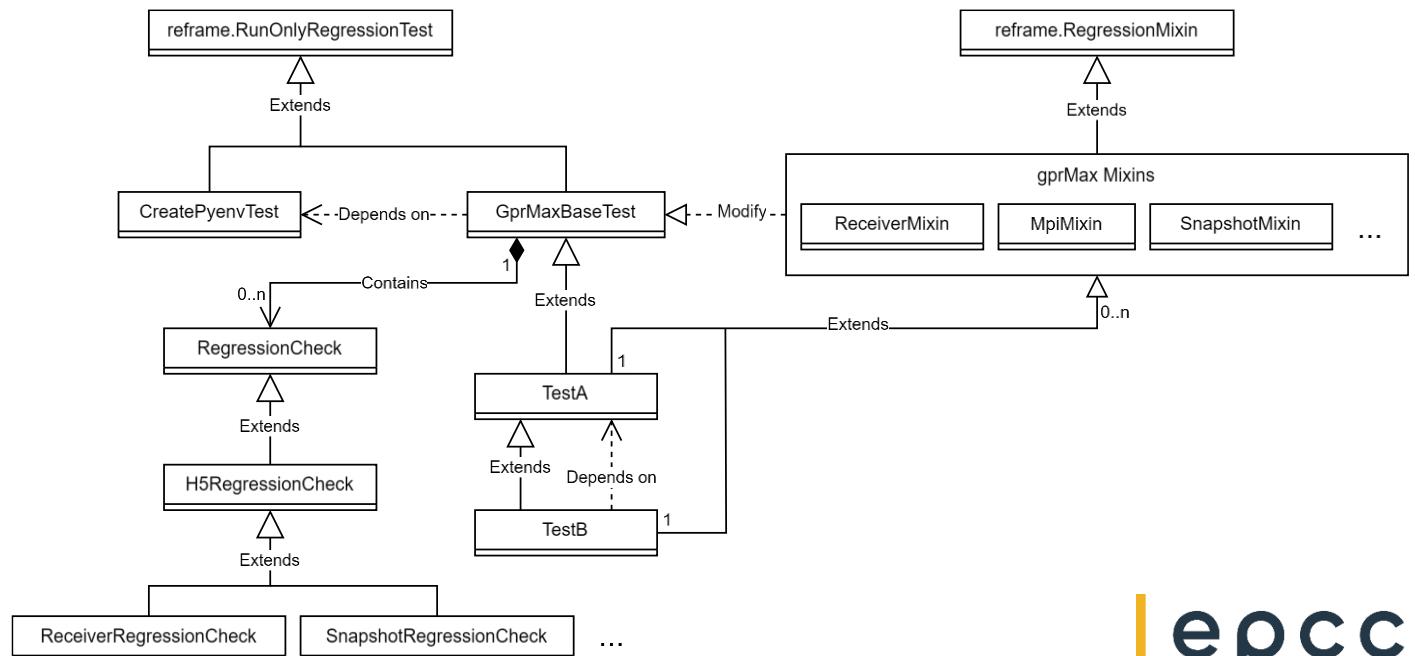


- HDF5 is well supported for HPC and Python
  - VTKHDF gives advantages of HDF5 while directly supporting visualisation
- 
- I/O performance effected by domain decomposition
  - Currently support independent I/O
    - Likely to get better write performance with collective I/O

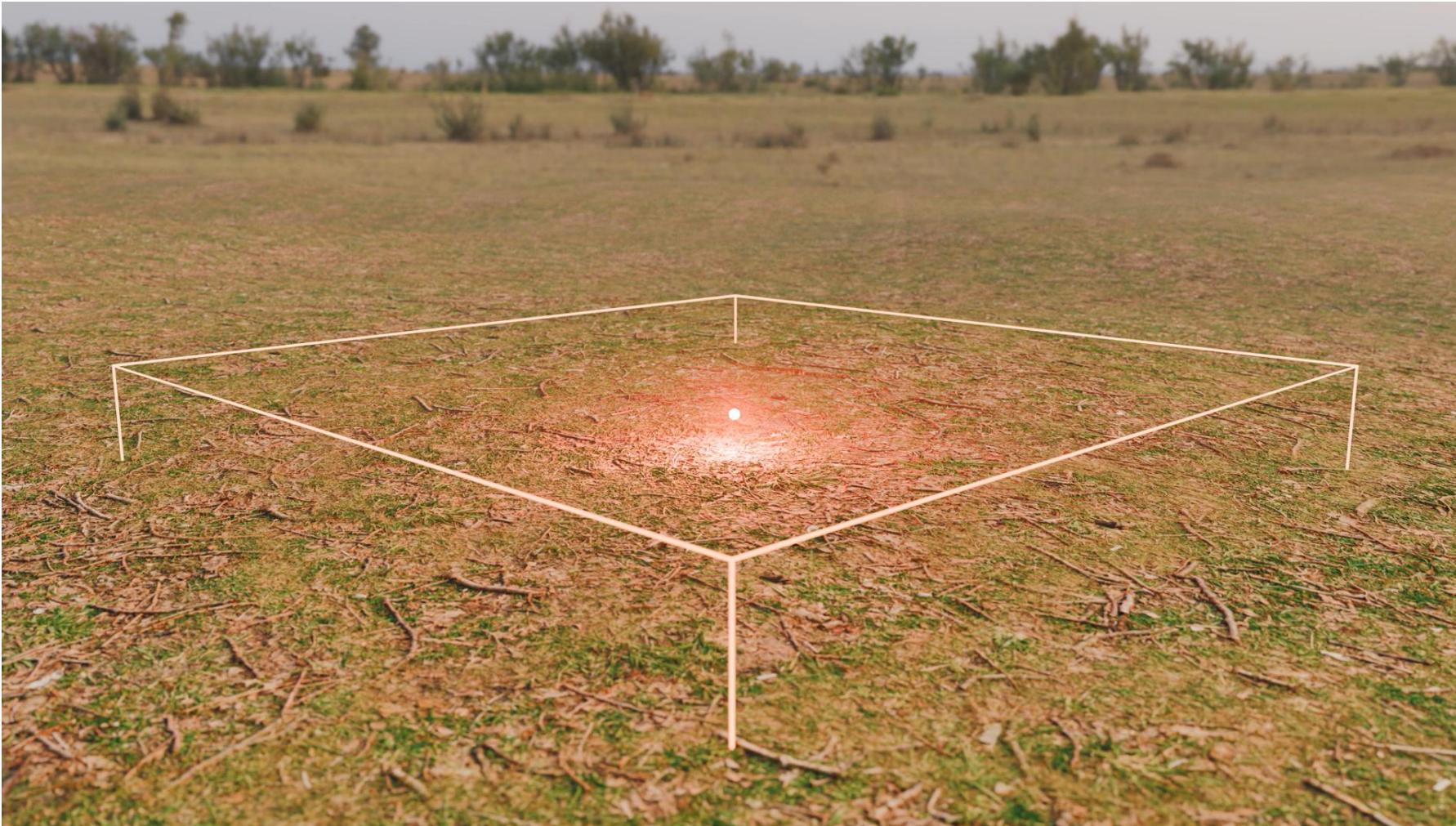
# Regression Testing with ReFrame



- Existing tests required manual inspection to check correctness
- Automated tests caught errors early
  - Full model regression tests – not unit tests
  - Can directly compare results from non-MPI tests with MPI tests
- Adding a new test requires:
  - A model input file
  - Typically 4-8 lines of code



# gprMax Visualisation – Sébastien Lemaire



<https://www.epcc.ed.ac.uk/research/scientific-visualisations>

| epcc |

# Project Team

- Craig Warren
- Antonis Giannopoulos
- James Richings
- Nathan Mannall



This work was funded under the embedded CSE programme of the ARCHER2 UK National Supercomputing Service (<https://www.archer2.ac.uk>).

