

4384

# Computational EM Simulation of Microscopic Graphene-Based Electrophysiology Probe at 7T MRI: Acceleration Using a Huygens' Box-Based Approach

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## Synopsis

**Keywords:** In Silico, In Silico, Computational Electromagnetic Simulation, Huygen's Box, EEG-fMRI, Graphene-based Electrophysiology Probes, MR Compatibility and Safety

**Motivation:** Concurrent electrophysiological-fMRI acquisitions have provided important new neuroscientific data, although conventional EEG probes can pose significant data quality and RF heating-related challenges, especially at high fields.

**Goal(s):** To investigate the compatibility and safety in the MRI environment of novel graphene-based microscopic electrophysiological probes with unsurpassed recording capability.

**Approach:** Computational electromagnetic (EM) simulations were conducted using a Huygens' Box (HB) method to increase the efficiency and enhance the spatial resolution of multi-port methods.

**Results:** The HB method achieved a spatial resolution of 0.0001mm (through-plane) and 0.01mm (in-plane) within practical simulation times, demonstrating acceptable SAR increase in the vicinity of the probe.

**Impact:** This study provides evidence on the superior MR suitability of graphene-based probes compared to the current technology for concurrent EEG-fMRI acquisitions, offering the prospect of unprecedented characterization of brain activity which could lead to better diagnostic and therapeutic strategies.

## Introduction

Concurrent EEG-fMRI is a powerful technique that simultaneously records electrical brain activity and hemodynamic changes, providing valuable insights into normal and pathological brain states<sup>1</sup>. This combined approach aims to optimize data collection while ensuring patient safety. Integrating EEG and fMRI poses challenges, including metal-based artifacts from conventional EEG probes that distort MRI images<sup>2</sup>. Additionally, RF-induced heating in the vicinity of the EEG components and the static magnetic field introduces risks of displacement and torque represent important potential health risks<sup>3,4</sup>. Probes using Graphene Solution-Gated Field-Effect Transistors (gFET) allow high-fidelity DC-coupled brain signal recordings<sup>5,6</sup>. This study focuses on their suitability for the MR environment. Computational electromagnetic (EM) simulations are useful to evaluate the interactions between the graphene-based probes and the MRI fields. However, a major challenge is the lengthy simulation times using standard techniques (>1000 hours), partly due to the probes' microscopic (sub-micrometric) structure. Here we explore the use of a Huygens' Box (HB)-based approach to reduce computation times and improving spatial resolution compared to conventional methods<sup>7</sup>. Two probe designs were investigated: intra- and epi-cortical<sup>5,6</sup>.

## Methods

EM simulation analysis based on the finite-difference time-domain (FDTD) method was performed on a Windows 11 PC (3.00GHz, 32GB RAM, Nvidia RTX 4090 GPU) using the aXware kernel on Sim4Life (V8.0, ZMT, Switzerland) in a 3-dimensional (3D) rodent model consisting of 68 tissues<sup>8,9</sup>.

- Simulation setup: 300 MHz of Gaussian excitation with a bandwidth of 625 MHz was used as the excitation source in both methods:  
(1) Multi-port method: Same excitation source in a two-port configuration, followed by impedance matching and combining the results in circular-polarized mode.  
(2) HB method: Two-step simulation. The first simulation is performed with the RF coil excited in circular-polarized mode, generating fields in a rectangular region of interest known as the Huygens' box, without any object (i.e. rodent/probe). The second simulation uses the Huygens' box as a source with the 3D rodent model placed inside the box, with and without the probes.
- RF coil modelling: A quadrature birdcage RF coil is used, with each rung (width: 9.9 mm) containing a capacitor (13.8 pF) placed on the end rings (width: 11.5 mm) to resonate at 300 MHz (Fig. 1A).
- Probe modelling: The 3D probe models were generated from 2D drawings and exported to individual layers via Rhino (V8, Washington, DC, USA) and finally converted to multi-layered 3D model in Sim4Life. Figure 2 shows the probe models.
- Estimated EM fields: Transmit RF field ( $B_1^+$ ), mass-averaged, and peak spatial-averaged specific absorption rate (SAR) averaged over 0.01 g, 0.1 g, and 1 g tissue mass were calculated following IEC guidelines<sup>10</sup>.

## Results

Table 1 shows the computational times for different simulation types and their respective grid sizes. Note the higher resolution and shorter simulation times for the HB method. Figure 3 displays  $B_1^+$ -field distributions in the rodent model for both multi-port and HB simulations, highlighting the similarity between the results and improved resolution for the latter.  $B_1^+$  magnitudes elevated by approximately 15–20% in the vicinity of the probes due to induced currents in the probe's metal layers during transmission. Figure 4 shows the SAR distributions in the rodent model for both multi-port and HB simulations, revealing elevated SAR near the probe. Mass-averaged SAR and peak spatial-averaged SAR values in the rodent model are presented in Fig. 4C.

## Discussion

The HB approach enhances EM simulations by improving computational efficiency and enabling higher-resolution field calculations around probes and the rodent model. However, a limitation is the inability to apply RF coil matching in HB simulations as effectively as in multi-port simulations, introducing slight uncertainties. SAR elevation in the vicinity of the graphene-based probes is modest.

## Conclusions

This study successfully demonstrates the estimation of EM interactions of graphene-based EEG probes within an MRI environment using the HB approach to accelerate simulations of these microscopic probes, which would otherwise be excessively long on a single GPU. Our simulations showed that the impact of the graphene-based probes on RF transmission and SAR deposition is modest, thereby satisfying a necessary requirement for their suitability for the MR environment. Further work is needed to optimize computational efficiency, conduct experimental verification using phantoms and evaluate the probe's electrophysiological performance in the MRI environment.

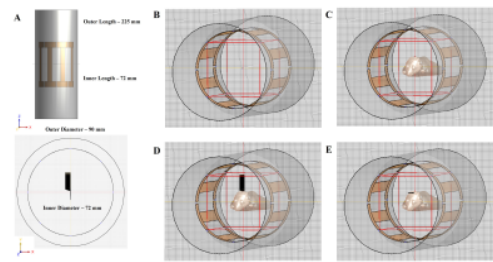
## Acknowledgements

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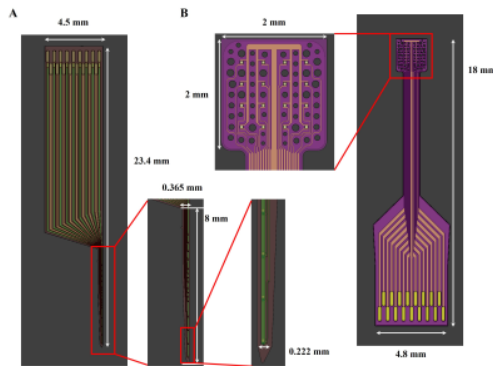
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Figures



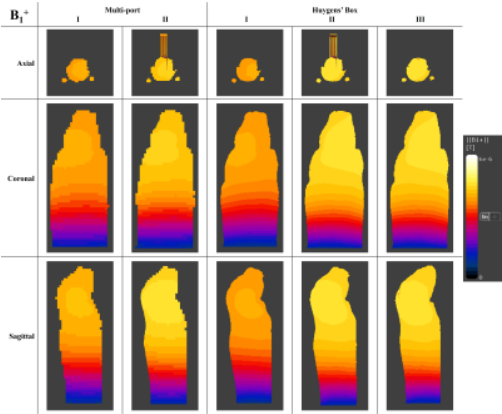
**Figure 1.** (A) Model of the 8-rung high-pass birdcage RF coil; Huygens' box approach: First step: creation of the Huygens' source, (B) with the RF coil acting as the source and the red box indicating the region of interest for the Huygens' box; Second step: Implementation of the Huygens' source with the rat and probe models placed inside the Huygens' box; (C) Rat model (without probe); (D) Rat model with intracortical probe; (E) Rat model with epicortical probe.



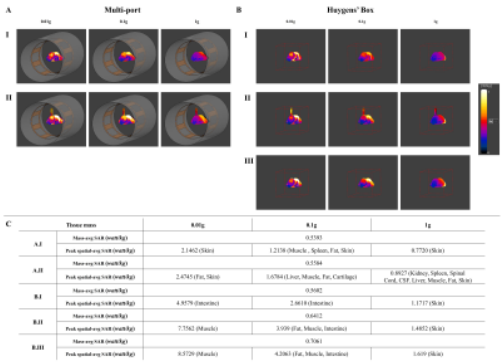
**Figure 2.** Schematic diagrams and dimensions of the probes: (A) Intracortical; (B) Epicortical. For a detailed description of the probes, please refer to [5, 6]. Due to Sim4Life limitations in simulating graphene's atomic monolayer thickness, a minimum thickness of 100 nm was implemented in this work.

| Multiport<br>Rat                                                                 | Multiport<br>Rat + probe 1                                                                                                   | Huygens' Box<br>Source Creation                                                               | Huygens' Box<br>Rat                                                                            | Huygens' Box<br>Rat + probe 1                                                                                                                | Huygens' Box<br>Rat + probe 2                                                                                                             |
|----------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
|                                                                                  |                                                                                                                              |                                                                                               |                                                                                                |                                                                                                                                              |                                                                                                                                           |
| Grid Size = 10 MCalls<br>- Rodent = 2 mm²<br>- RF coil = 1 mm²<br>Run time = 1hr | Grid Size = 40.5 MCalls<br>- gPCT = 0.01 x 0.01 x<br>- 0.0001 mm²<br>- Rodent = 2 mm²<br>- RF coil = 1 mm²<br>Run time = 450 | Grid Size = 17.5 MCalls<br>- RF coil = 1 mm²<br>- Huygens' box = 1<br>mm<br>Run time = 30 min | Grid Size = 20 MCalls<br>- Rodent = 0.25 mm²<br>- Huygens' box = 0.25<br>mm²<br>Run time = 1hr | Grid Size = 70.5 MCalls<br>- gPCT = 0.01 x 0.01 x<br>- 0.0001 mm²<br>- Rodent = 0.25 mm²<br>- Huygens' box = 0.25<br>mm²<br>Run time = 200hr | Grid Size = 61 MCalls<br>- gPCT = 0.0001 x 0.001<br>x 0.01 mm²<br>- Rodent = 0.25 mm²<br>- Huygens' box = 0.25<br>mm²<br>Run time = 140hr |

**Table 1.** Comparison of grid size and computational run time for each type of simulation performed in this study. Note that multi-port simulations could not be run with the same grid size as the HB approach on a single GPU. To highlight the benefits of the HB approach, only simulations with higher resolutions are shown here.



**Figure 3.** Simulated  $B_1^+$  field distribution in the rodent model for the multi-port approach: (I) without and (II) with intracortical probe; and for the HB approach: (I) without, (II) with intracortical, and (III) with epicortical probe models in axial, coronal, and sagittal views. Values normalized to an input power of 1 watt.



**Figure 4.** Simulated mass-averaged SAR distribution in the rodent model for (A) multi-port approach: (I) without and (II) with intracortical probe; (B) HB approach: (I) without, (II) with intracortical, and (III) with epicortical probe models for 0.01g, 0.1g, and 1g tissue mass; and (C) mass-averaged SAR and peak spatial-averaged SAR values for the specified simulation approaches. Values normalized to an input power of 1 watt.