LA-UR-18-29614
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Intended for: Report

Issued: 2018-10-10

Evaluating the Feasibility of MCNP/FDTD EMP Calculations at Altitudes above 20km

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Abstract

This report investigates the use of MCNP/FDTD for 2D EMP calculations at altitudes above 20km. The objective is to determine the feasibility of performing EMP calculations for high altitude nuclear detonations using the MCNP/FDTD codes. The work in this report indicates that the issue with running such EMP calculations lies more in MCNP than in FDTD. In general, when performing EMP calculations with MCNP/FDTD, the majority of the computation time is in getting the results from MCNP. Typically, for EMP calculations with spatial domains of about 5 to 10km in both the x and z directions, the MCNP calculations take weeks to complete and the FDTD portion of the computation only takes one to two days. The problems with running MCNP on large problems are largely due to memory issues. One issue is that MCNP requires all tally grids of a simulation to reside in the memory of a single node (128GB on snow) and this, in turn, requires multiple MCNP simulations to complete large spatial/time domain problems. For the large spatial domain problems being considered in this report, the number of required MCNP simulations is more than one hundred. Another issue is the volume of output data from MCNP is enormous since the tally grids have traditionally been of one shake time resolution and 5m by 5m spatial resolution. The FDTD input file sizes for a 60km height-of-burst (HOB) simulation is likely to be over 100TB for 300 microseconds of tally data and these high altitude simulations could require 800 microseconds to model the neutron transport and interactions with the atmosphere. This report will provide an approach to overcome the issues associated with running MCNP on large problems. As part of this work, FDTD was also run over very large spatial domains using artificially generated input data. The results of running FDTD on these large problems indicate that FDTD would not have problems with a spatial domain as large as 60km by 90km. A FDTD simulation for a 60km HOB scenario and a spatial domain of 60km by 90km ran on 30 nodes (snow) and finished at a simulation time of 7 microseconds after 12 hours of wall clock time (snow). In order for FDTD to run on this large problem, the code had to modified to more efficiently read data in from the input file.

1 Overview

This report investigates the use of MCNP/FDTD for 2D EMP calculations at altitudes above 20km. The objective is to determine the feasibility of performing EMP calculations for high altitude nuclear detonations using the MCNP/FDTD codes. The work in the report indicates that the challenges with running such EMP calculations occurs mostly in MCNP and not in FDTD. There are several reasons why there are challenges with running MCNP over large spatial domains. One issue is that MCNP requires that all of the mesh tally grids reside in the memory of a single HPC node. This forces the spatial and time domain for the tally grids to be broken up into sub-grids and completed with separate MCNP simulations. For the large spatial domain problems being considered, the number of MCNP runs could be in the hundreds. Managing, executing, and getting the necessary computational time for all of these MCNP runs could be challenging. Another issue with running MCNP on these problems is in data management as the files generated by MCNP and the input files for FDTD can become enomorous. As will be discusssed in the next section, running MCNP out to 300 microseconds for a 60 km height-of-burst (HOB) and a spatial domain of 60km by 90km could require more than 100TB of input data for FDTD. To capture all of the relevant physics, the MCNP simulations for neutron output may have to run out to 800 microseconds. The estimate of 800 microseconds is based on the probability of neutrons interacting in the thin air and by computing the column density from a 60km HOB to various locations in space. Thus, in order to make these runs reasonable, the resolution of the MCNP tally grids need to be reduced. Later in this report, a strategy is given where the time resolution is decreased during time regions when there is less activity.

In the case of FDTD, this feasibility study indicates that running FDTD on very large domains is not too time prohibitive. The FDTD simulations discussed in this report used artificially generated input data. Section 3 on FDTD results will provide more details on the method for generating the input files for FDTD. The largest FDTD spatial domain problem run in this study was 60km (radially) by 90km (height) and, using 30 nodes (snow), this problem ran out to more than 7 microseconds in 12 hours of wall clock time. In another simulation, FDTD ran out to 22 microseconds with 30 nodes on a problem with a FDTD spatial domain of 30km by 61km.

FDTD had to be modified to run on these large problems. The subroutine read-awe-data-file() of the FDTD code that reads in the input file had to be changed to be more memory efficient. In the original FDTD code, the function read-awe-data-file() was creating four arrays of size nx by ny (where nx and ny are the number of spatial cells in the input file and MCNP simulation) for every process. The intent of the function read-awe-data-file() is for the process with rank zero to read the input file and broadcast the data to the other processes. The subroutine read-awe-data-file() was modified so that the arrays of size nx by ny are only created for the process with rank zero. Prior to making this modification, FDTD would crash when attempting to run problems with spatial extents of about 30km or more. After the modification, FDTD successfully ran on a spatial domain as large as 60km by 90km.

One possible way to proceed with the MCNP runs is to reduce the time resolution of the tally grids for neutron simulations at times when there is not much changing in terms of the energy deposition rate (E_{dr}) and electron current density (J_e). The energy deposition rate and electron current density at each spatial and time point is the provided input to FDTD. In the case of photons, it should be sufficient to tally data for 30 microseconds (3000 shakes) at each spatial location. That is, tally data at each point in space would begin at time of first light and then end 30 microseconds later. It will take about 60 MCNP simulations to capture E_{dr} and J_e due to the photon source. See the next section for more information. In the case of neutrons, the problem is more challenging since the slower moving neutrons interact with the atmosphere and generate ionizing photons. Also, since the air has such low density at high altitudes such as 60km, the neutrons can travel quite far before their energy is reduced low enough so that they do not have to be modeled. It is possible that neutron transport would have to be modeled for 20 to 40 km and this would require tally data for 400 to 800 microseconds. Tallying data for 400 to 800 microseconds will require too many MCNP simulations if the tally grid resolution is kept at one shake. One possibility is to significantly reduce the time resolution of the tally grids for times when the energy deposition rate and electron current density is slowly varying. If the time resolution is decreased to 10 shakes at times when E_{dr} and J_e are slowly varying (which should be the vast majority of time) then 800 microseconds of tally data could be obtained with about 150 MCNP simulations. Furthermore, it may be possible to further reduce the number of MCNP runs since 800 microseconds of tally data may not be necessary for the neutron source at all spatial locations. The next section will provide some more details and an estimate of the amount of run-time required for all of these MCNP simulations. To generate the FDTD input file, the MCNP results are time convolved with the source's time profile. When performing the time convolution step for these MCNP simulations, the MCNP grid at ten shakes will be interpolated to a one shake grid and the FDTD input file will be written at one shake resolution.

Prior to running the neutron MCNP simulations, a quick simulation study will be undertaken to examine the behavior of E_{dr} and J_e at various points in space. For example, the tally grids could be set up to capture data at altitudes of 5km, 15km,..., 85km, for all locations radially, and for a total of 800 microseconds or more. That is, a tally grid will be defined for each of the heights h = 5km ,15km,..., 85km to be a single zone vertically and for all locations radially (0 to 60km). All of these tally grids can be specified in a single MCNP simulation. This MCNP simulation would be used to justify the use and location of a lower resolution time grid in the full domain MCNP simulations.

2 Analysis of Large MCNP Runs

This section will provide a short analysis of the number of needed MCNP runs and the corresponding required computational time to obtain reasonable results for a 60km HOB scenario and tally grids extending 60km radially and 90km above the ground. MCNP runs consist of separate simulations for the photon source and the neutron source. Since photons travel at the speed of light, the time required to tally the energy depostion rate (E_{dr}) and electron current density (J_e) is less as compared to neutrons which travel at about 1/6th (or less) of the speed of light. Past experience has indicated that the photon simulations only need to be tallied for 30 microseconds. Assuming that each spatial cell in the tally requires 30 microseconds of tallies, the amount of memory for the photon MCNP tallies is

$$M_p = 12 * 12000 * 18000 * 3000 = 7.1TB. \tag{1}$$

The constant twelve in the above equation is due to floating point precision used for E_{dr} an J_e. The variable J_e is a 2D vector for the 2D simulations considered in this report. Since each node on snow has 128GB of memory, the number of separate photon source MCNP simulations is 57. The number of runs could be reduced by noting places in time where the variables E_{dr} and J_e are slowly varying and then reducing the MCNP tally grid time resolution.

For the neutrons, significantly more MCNP runs are needed. The neutrons travel at about 1/6th the speed of light, or less, and generate ionizing photons as they interact with the atmosphere. Therefore, tally grids for each spatial location must start at the time is takes light to travel to that point and continue until much later in time. Based on computations of the column density, the neutrons may have to be modeled for 800 microseconds. In order to get data for 800 microseconds, the tally grids must have their resolution lowered. The plan is to use a high resolution time grid around times at which E_{dr} and J_e have a high rate of change and use much lower (10 sh) resolution at other times. Under the cirumstance where the tally grids have to be at high time resolution for 30 microsecods and low resolution for 800 microseconds, the number of MCNP runs would be about 210 (about 60 for the high resolution grid data for neutrons and 150 for the low resolution grid). The number of runs for the low resolution neutron source grid is obtained from equation one above with the number of time zones at 8000 (instead of 3000) and then dividing the result by 128GB.

Table I: MCNP Simulations

Desc.	t res.	No. MCNP runs	nodes/run	node · hours	Elapsed Time
Photon	1 sh	57	5	14250	12 days
Neutron	1 sh	57	5	14250	12 days
Neutron low	10 sh	152	10	76000	63 days

Table I provides a summary of the MCNP runs and an estimate of the computational resources that would be used for the runs. In table I, the column labeled ”t res.” is the time resolution of the MCNP tally grids. The number of nodes per run provided in the table is an estimate based off of previous simulations. The number of node · hours is based on 50 hours of wall clock time for each of the MCNP runs using the number of specified nodes per run. The elapsed time is an estimate of the amount of ”calendar” time it would take to get the simulation results completed. The results are based off of having access to 1200 node · hours (100 nodes for 12 hours of 50 nodes for 24 hours) per day to perform these calcuations.

Another issue with running MCNP on these large spatial domain problems is the size of generated the FDTD input files. For a spatial domain of 60km by 90km in MCNP and a 60km HOB, the projected FDTD input file size for 100, 200, 300, and 800 microseconds of tallies is 6TB, 44TB, 112TB, and 466TB. However, it is also possible to run FDTD in stages and only provide the data for the needed times of the current FDTD run. That is, a FDTD simulation can be run out to 100 microseconds using an input file with data from 0 to 100 microseconds, a second simulation can then follow with the input file having data from 100 to 200 microseconds, and, so on, until the FDTD simulation has ran to late enough in time.

3 FDTD Results

This section will provide some results on timing and the following section will give 2D snap shots from the FDTD results. The FDTD simulations consisted of very large spatial domains. Some of the different FDTD simulations that were attempted are listed in table II. All of the simulations consisted of MCNP input data at one shake resolution and covering times from 0 to 10000 shakes.

For the FDTD simulations, an artificial FDTD input file was generated. In all cases, the generated FDTD input file was of maximal size for the specified MCNP domain. In the current method of generating FDTD input files from actual MCNP results, zero values of energy deposition rate and electron current density are not written to the FDTD input file. Thus, data is only written for points (x,y,t) where the time for light to travel from the source location to (x,y) is greater than or equal to t. This same prescription was followed when the artificial FDTD input files were generated. Besides that, the generated artificial FDTD input files are of maximal size in that the energy deposition rate and electron current density are written for all (x,y,t) that satisfy the time of light travel restriction mentioned previously.

In table II, the column ”MCNP Domain” represents the spatial domain used when generating the FDTD input file. A zone resolution of 5m by 5m was used in the generation of the FDTD input file. Column labeled ”HOB” is the assumed height-of-burst of the source when generating the FDTD input file. The column ”File Size” gives the size of the corresponding FDTD input file. The ”FDTD Domain” is the spatial extents used in the FDTD simulation. All spatial information is listed as (x extent) x (y extent). The sixth column gives the number of nodes used in the simulation. All simulations were performed on snow (36 core per node, 128GB memory per node). The last column ”Sim. time” gives the simulated time in FDTD after running for 12 hours with the corresponding number of nodes.

The first run listed in the table is called ”0-data” and consists of setting the energy deposition rate and electron current density to zero at all points in space and time. The remaining listed input files for FDTD consisted of non-zero artificial data that were generated by assuming an exponential decay in space and time. The exponential decay in space was based on (or a function of) the computed column density from each point in space back to the source location. The exponential decay in time, which multiplies with the column density exponential decay, was based on the difference between the input time and the time of ”first light”. Reasonable initial values (i.e., when column density is zero and retarded time is zero) were selected for both electron current density and energy deposition rate.

The runs labeled ”Art. 1” and ”Art. 2” use the same input file for FDTD. Initialy increasing the MCNP domain size for the FDTD input file beyond the one used for ”Art. 1” and ”Art. 2” started to create issues. The FDTD program would crash and give an error message about running out-of-memory. The number of nodes were increased, up to 30 nodes in some cases, and FDTD would still crash even with a a modest increase in the MCNP domain size. This was an indication of an issue in the FDTD code since the problem did not appear to be simply due to not having enough nodes for the given simulation. The FDTD code was modified, as decribed in the first section, and recompiled. After modification, FDTD successfully ran on all problem sizes list in table II.

From the results of table II, running very large problems with extents of 60km by 90km appears to be fairly reasonable. Assuming that the results in the table for the 60km by 90km simulation scales linearly to 100 nodes, a 100 node simulation could reach 23 microseconds after 12 hours of wall clock time. Obtaining access to 1200 node $\cdot$ hours per day for this FDTD simulation would result in about 34 days of calendar time for the simulation to reach 800 microseconds.

Table II: FDTD Simulations

Name	HOB	MCNP Domain	File Size	FDTD Domain	# Nodes	Sim. time
0-data	18km	10km x 25km	1.96TB	12km x 25km	16	0-48μs
Art. 1	25km	15km x 35km	3.37TB	18km x 35km	16	0-37μs
Art. 2	25km	15km x 35km	3.37TB	30km x 35km	16	0-26μs
Art. 2 Restart	25km	15km x 35km	3.37TB	30km x 35km	16	26-46μs
Art. 2 Restart	25km	15km x 35km	3.37TB	30km x 35km	16	46-60μs
Art. 3	60km	60km x 90km	6.17TB	30km x 61km	30	0-22μs
Art. 4	60km	60km x 90km	6.17TB	60km x 90km	30	0-8μs

4 Imagery

This last section is effectively an appendix with 2D snap shot images from some of the FDTD simulations. Each subsection will provide a list of images from a single simulation.

4.1 25 km HOB, Artificial MCNP Data

In this subsection, 2D snap shots are given for a 25 km HOB FDTD simulation. This is the ”Art. 1” simulation of table II. The FDTD simulation extended radially out 18 km and up to a height of 35 km.

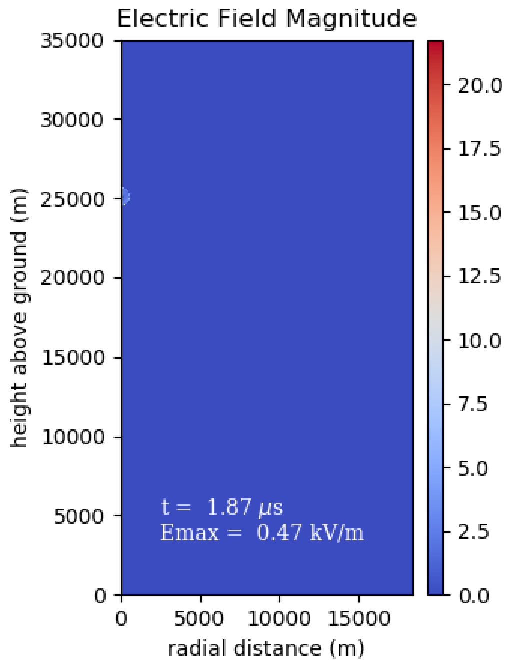

Figure 1: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

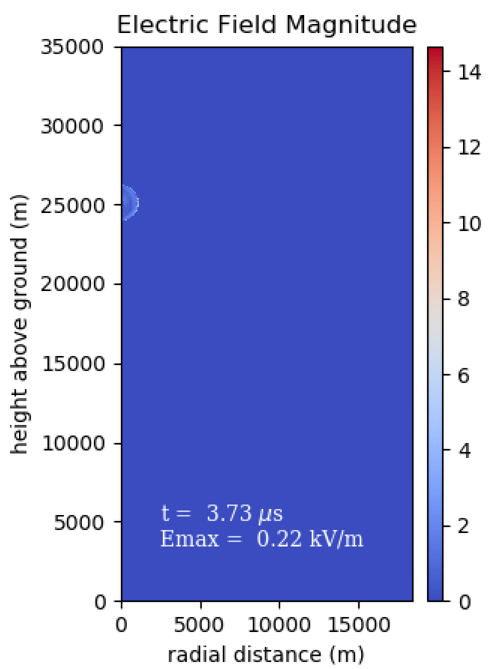

Figure 2: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

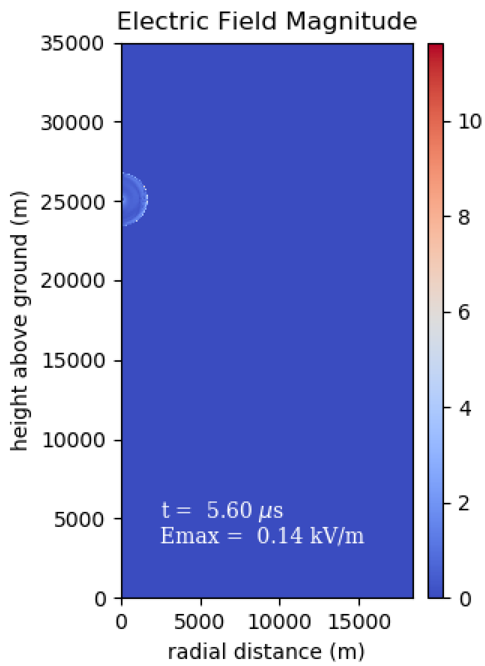

Figure 3: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

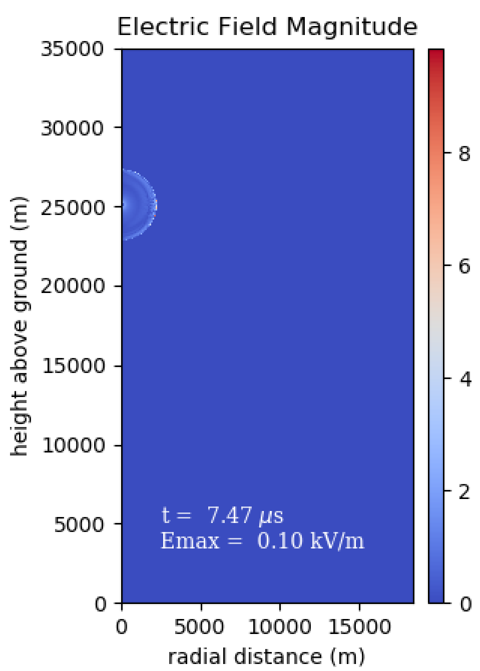

Figure 4: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

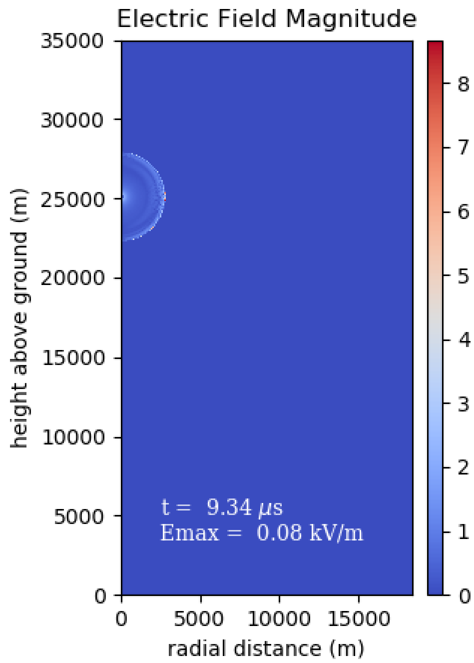

Figure 5: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

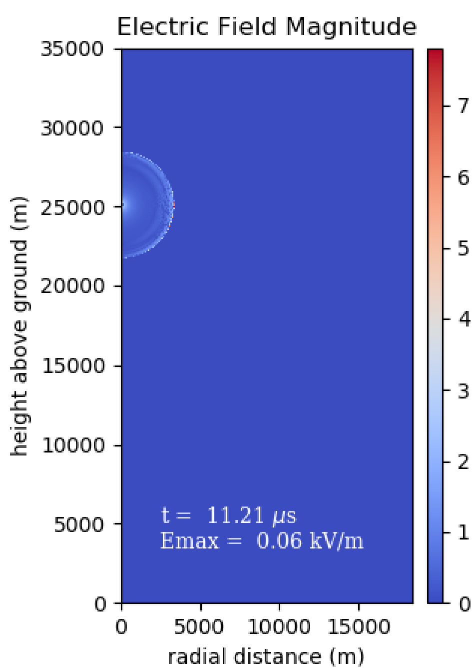

Figure 6: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

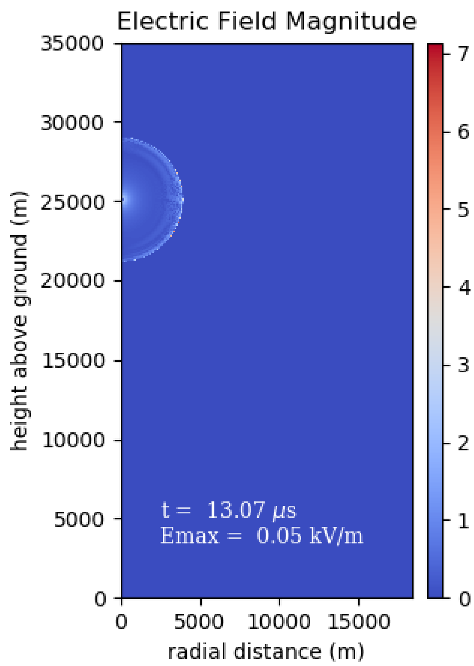

Figure 7: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

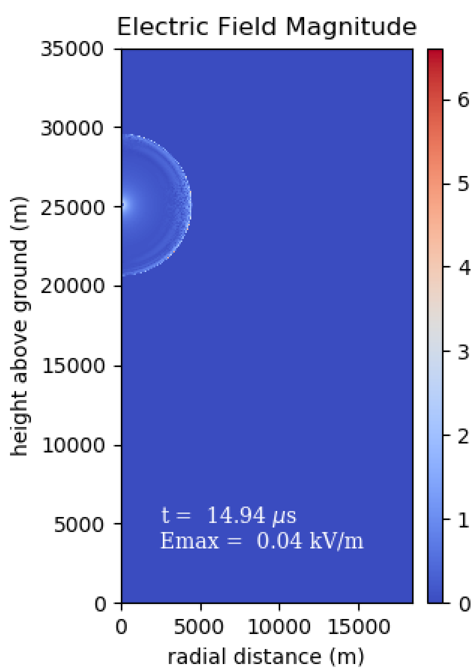

Figure 8: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

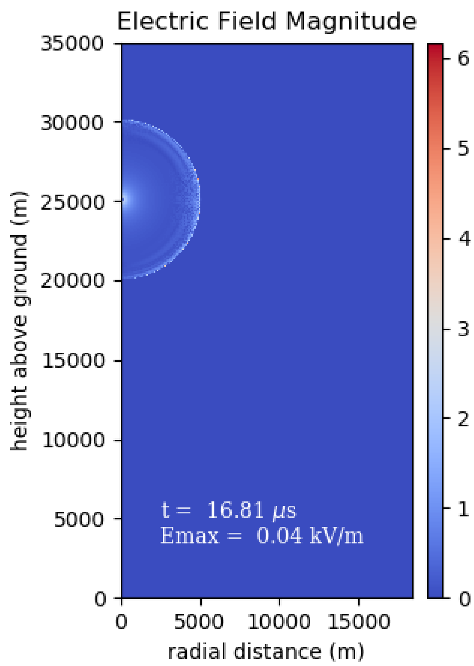

Figure 9: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

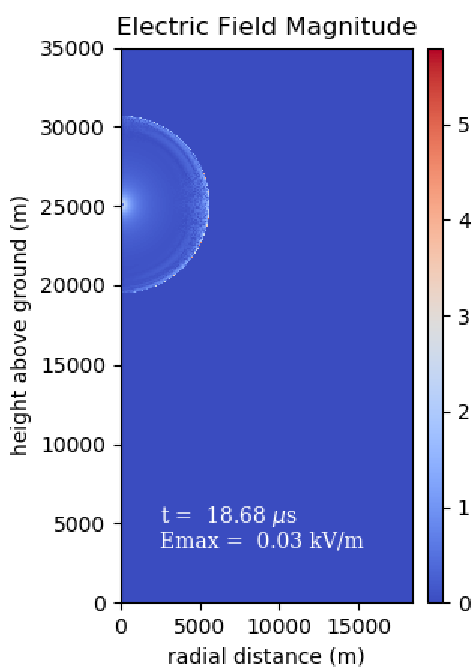

Figure 10: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

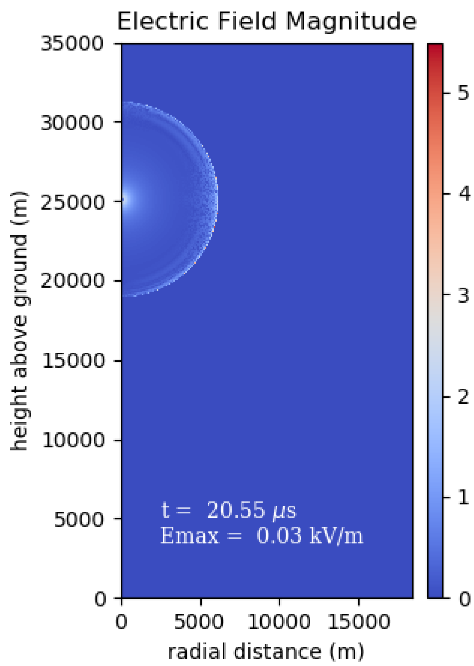

Figure 11: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

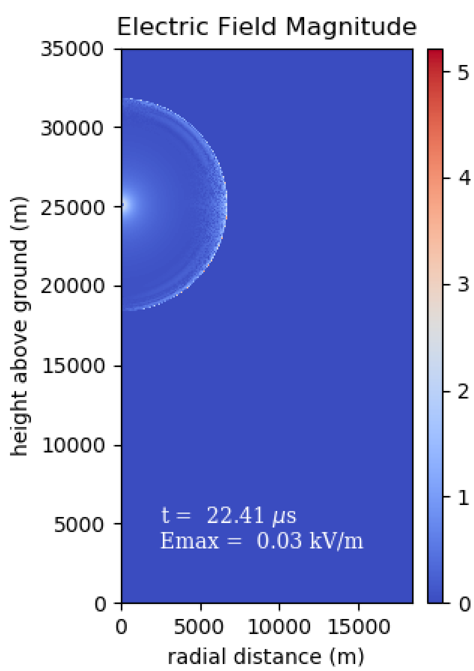

Figure 12: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

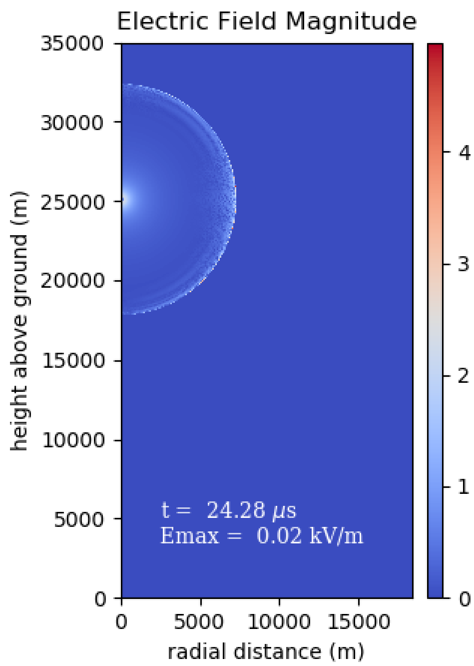

Figure 13: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

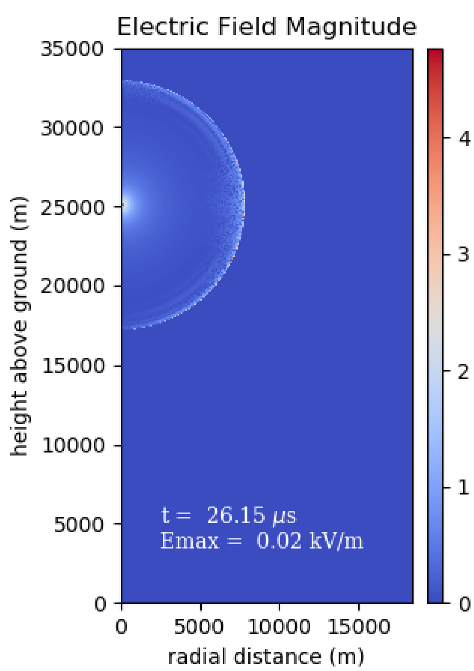

Figure 14: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

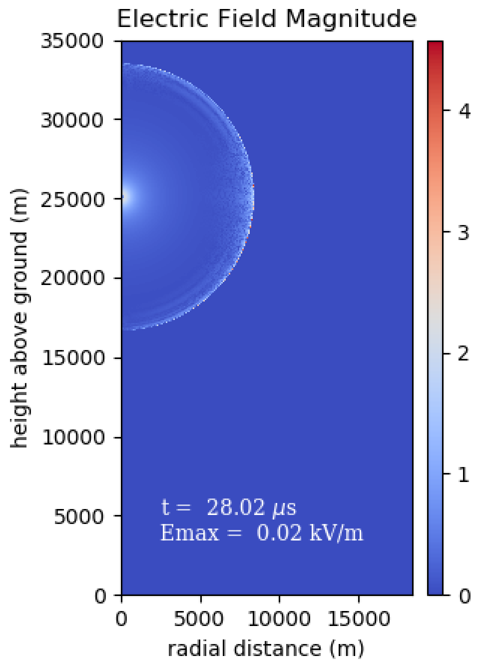

Figure 15: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

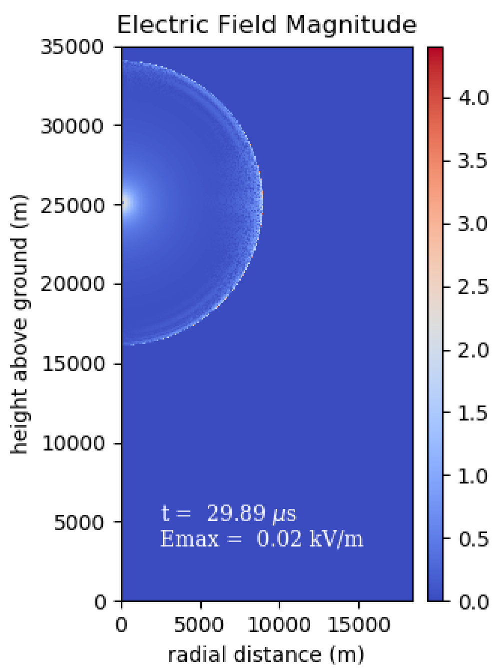

Figure 16: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

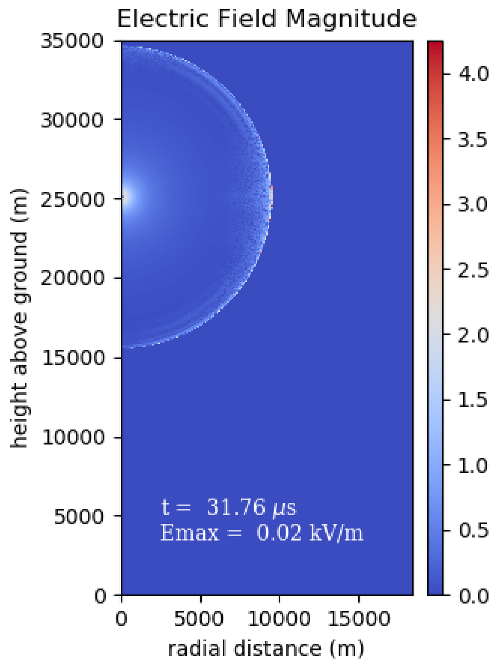

Figure 17: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

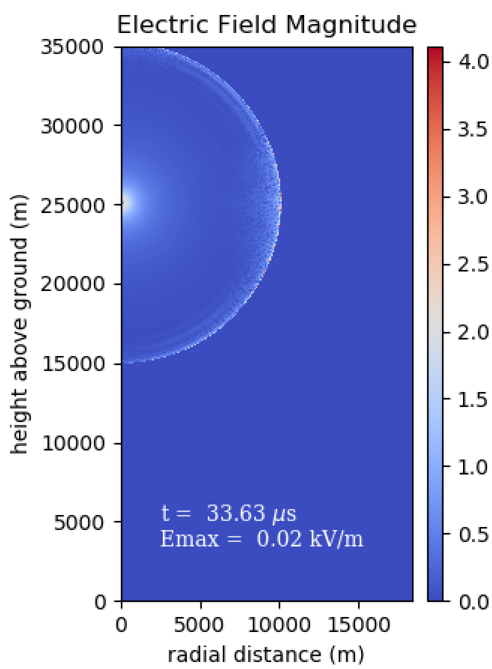

Figure 18: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

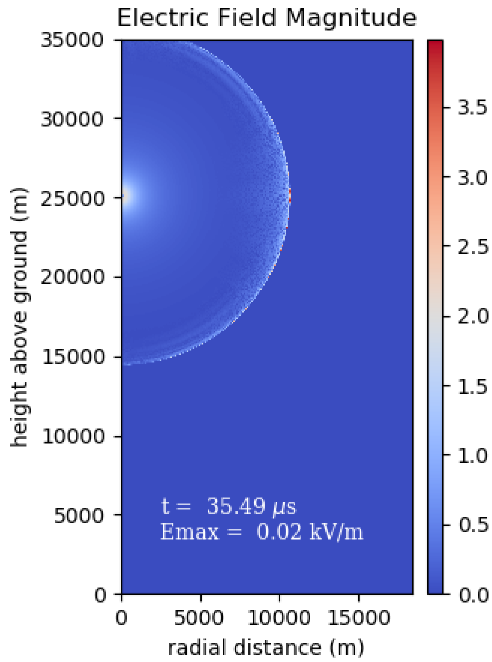

Figure 19: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

4.2 25 km HOB, Artificial MCNP Data, FDTD extended radially

In this section, 2D snap shots are given for a 25 km HOB FDTD simulation. The FDTD simulation extended radially out 30 km and up to a height of 35 km.

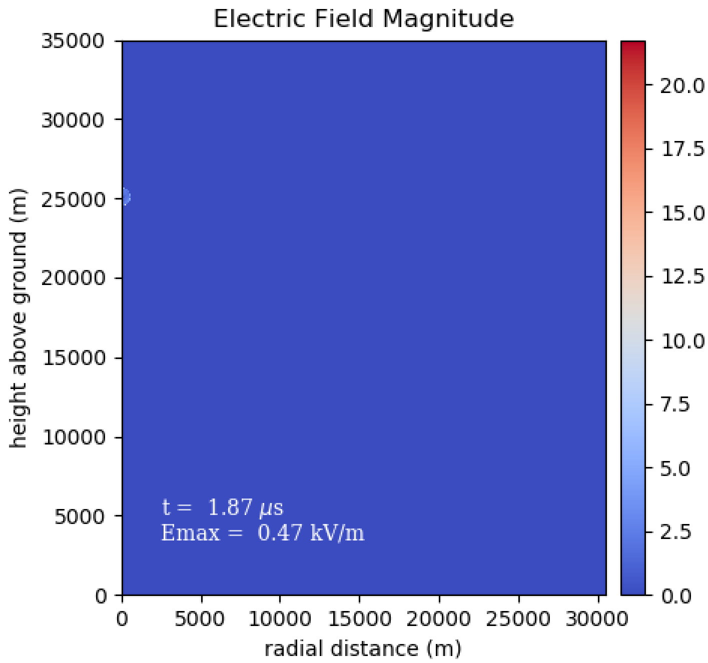

Figure 20: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

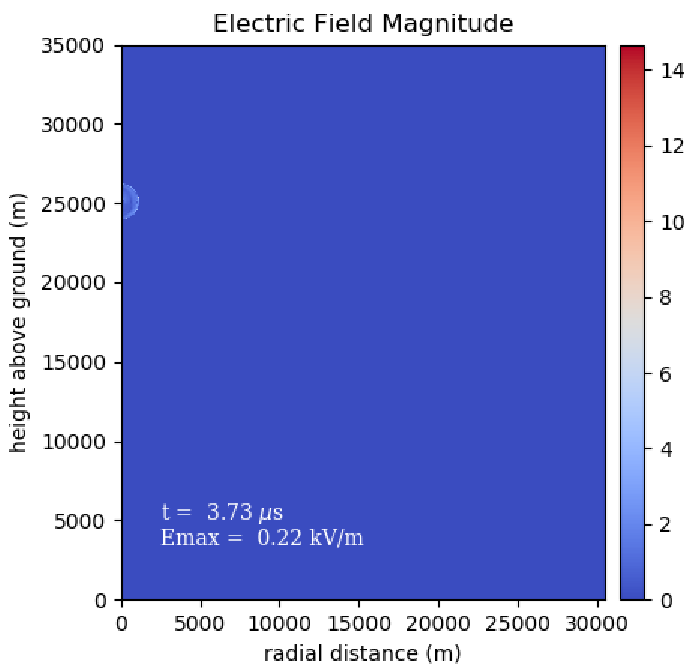

Figure 21: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

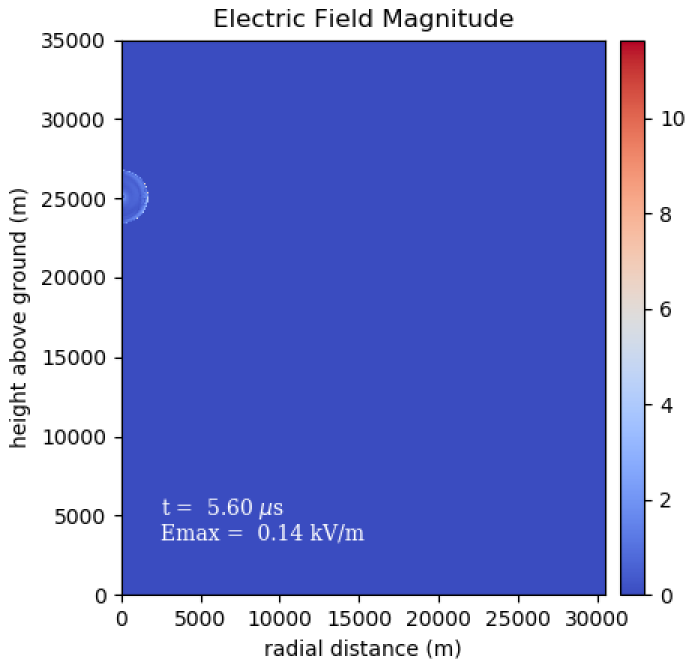

Figure 22: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

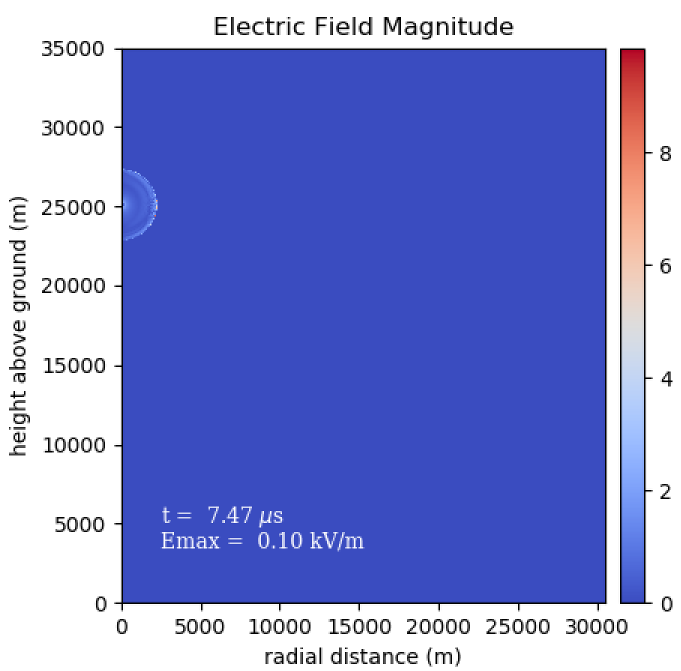

Figure 23: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

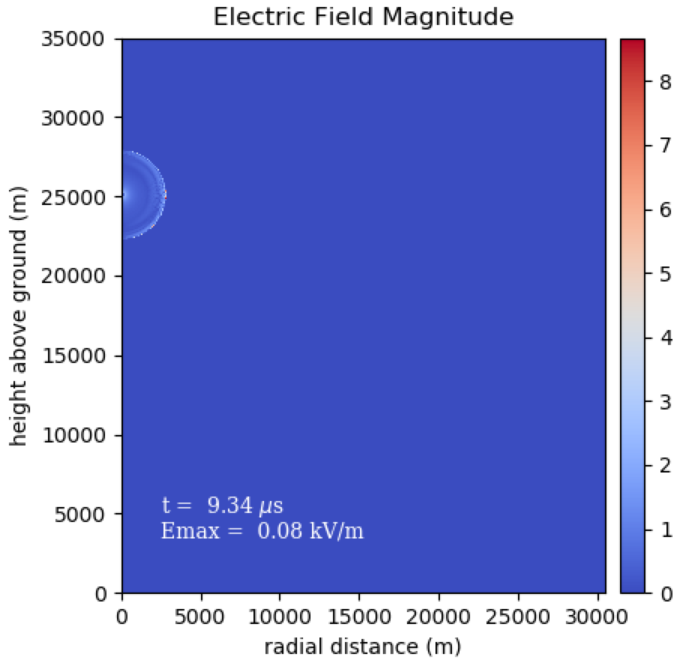

Figure 24: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

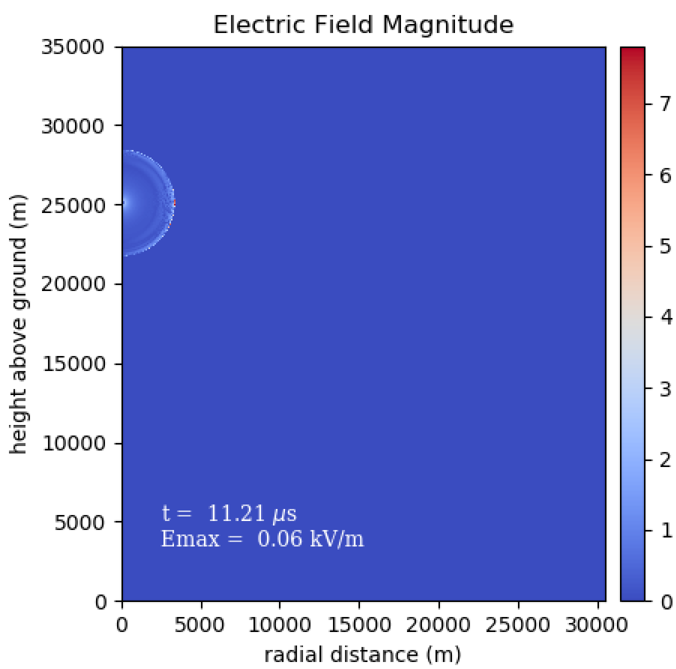

Figure 25: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

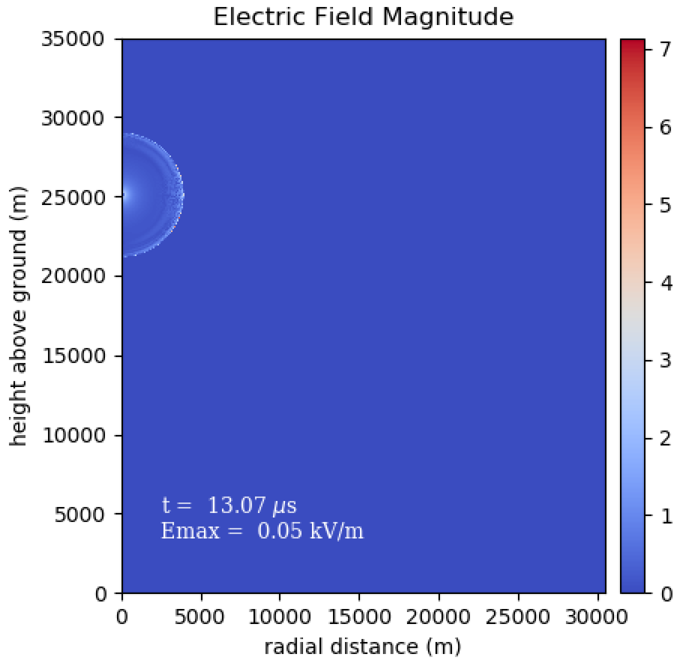

Figure 26: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

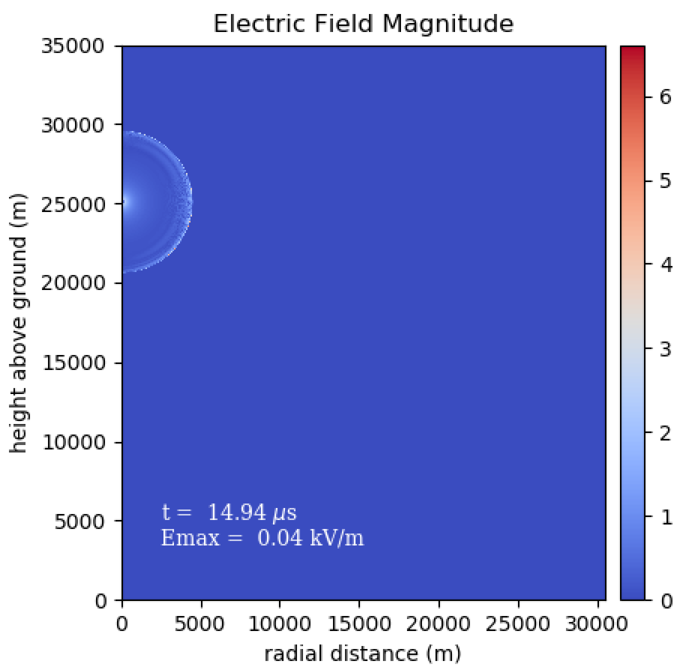

Figure 27: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

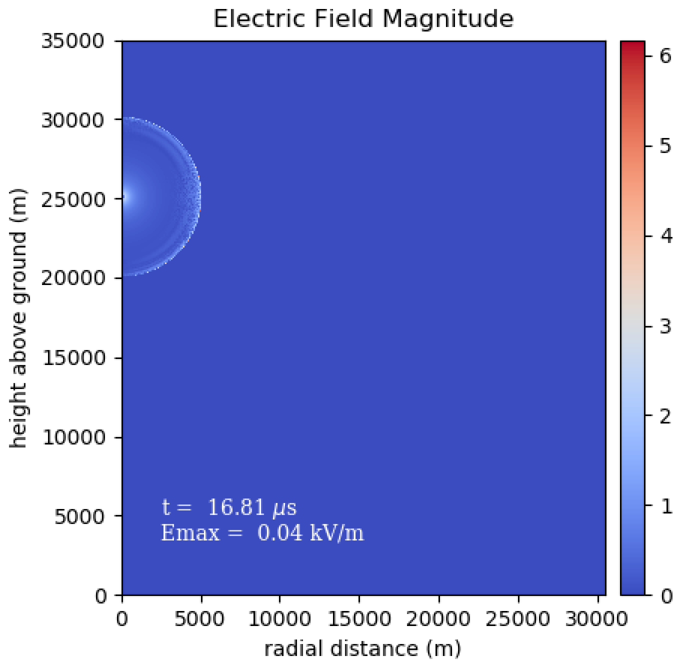

Figure 28: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

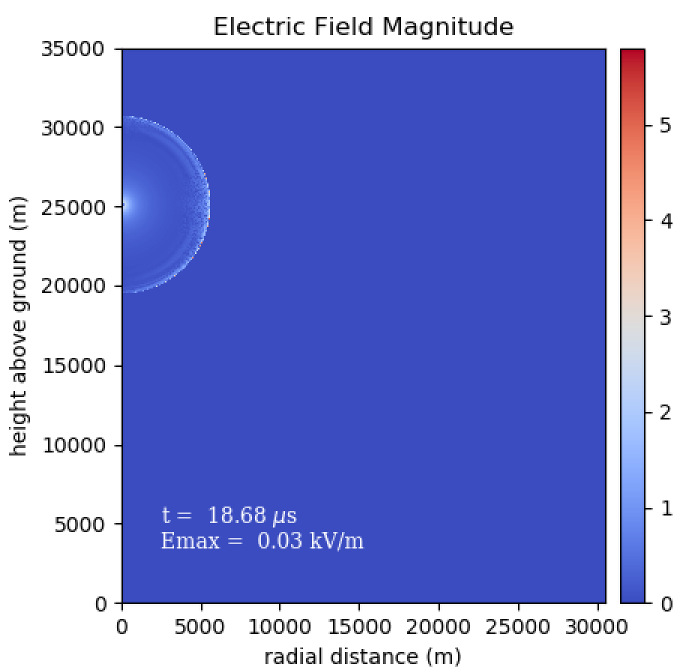

Figure 29: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

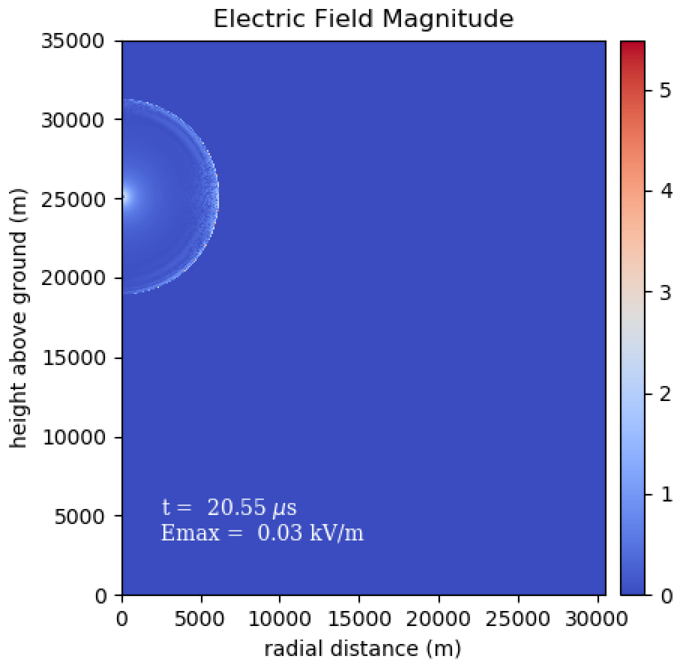

Figure 30: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

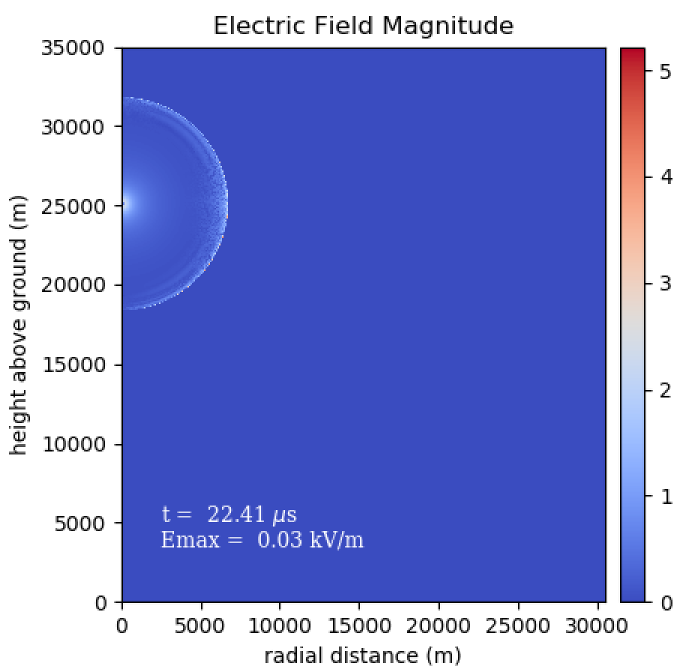

Figure 31: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

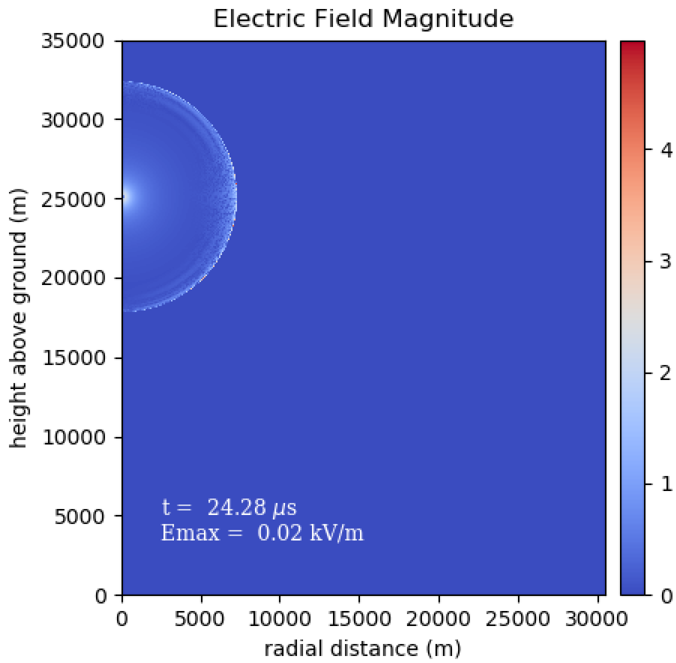

Figure 32: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

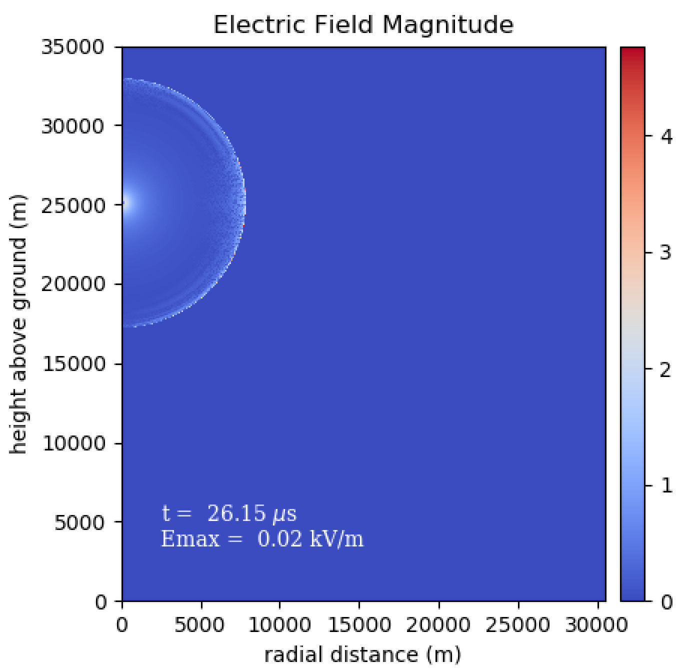

Figure 33: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

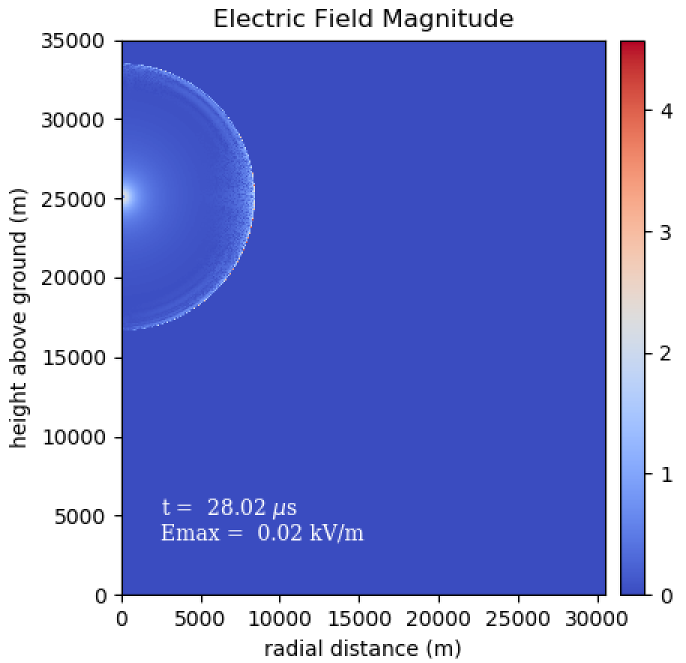

Figure 34: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

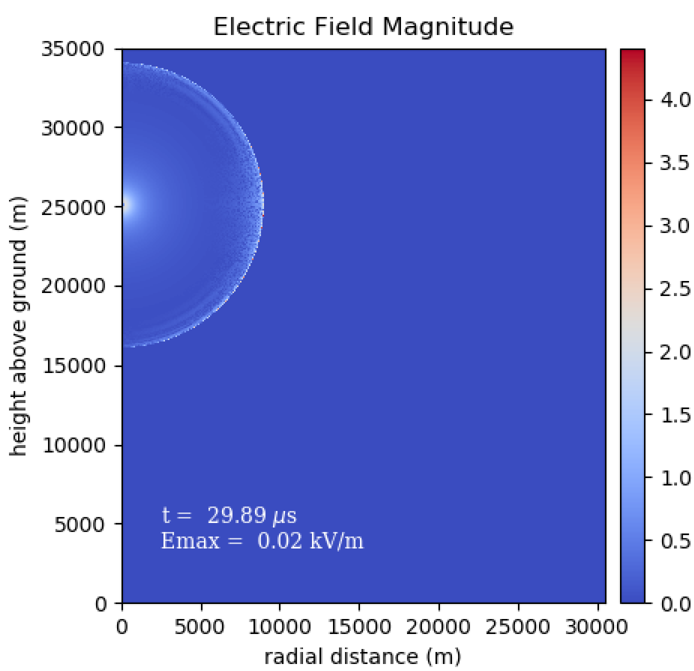

Figure 35: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

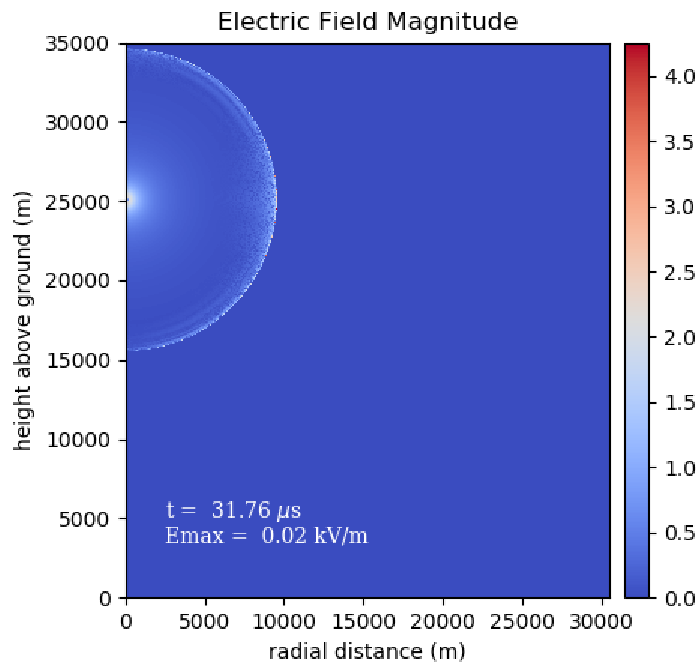

Figure 36: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

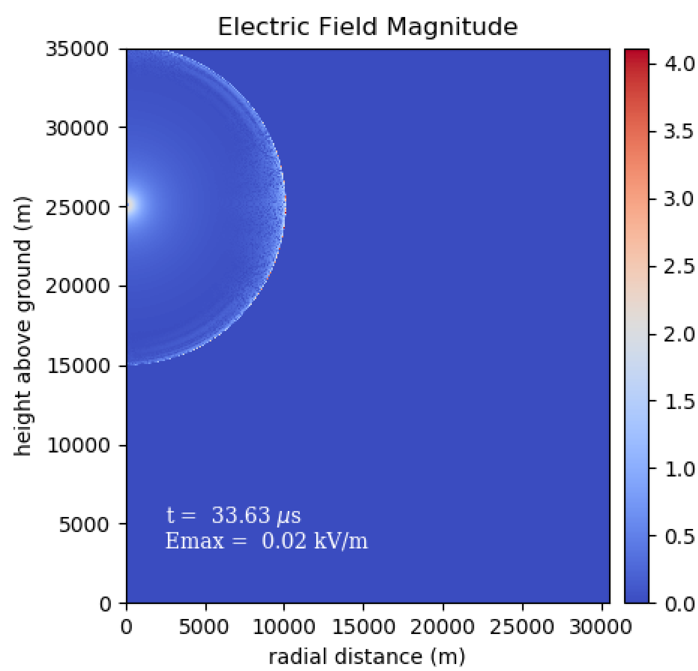

Figure 37: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

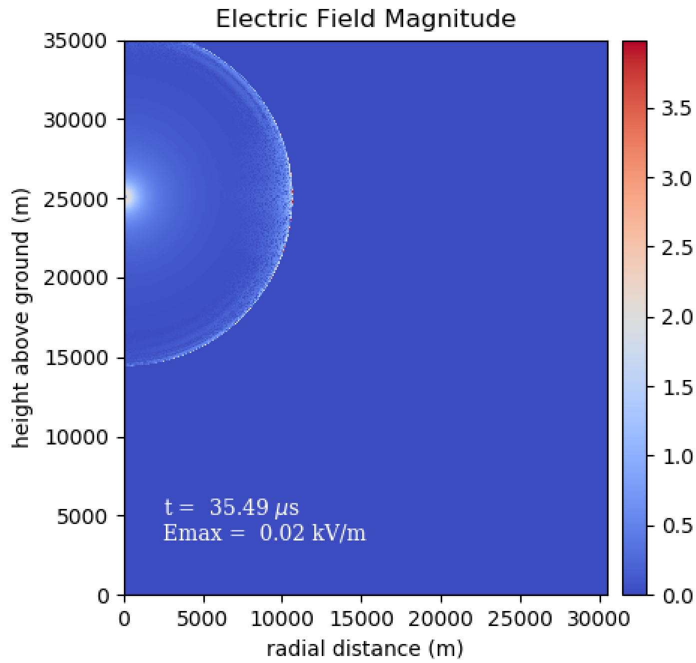

Figure 38: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

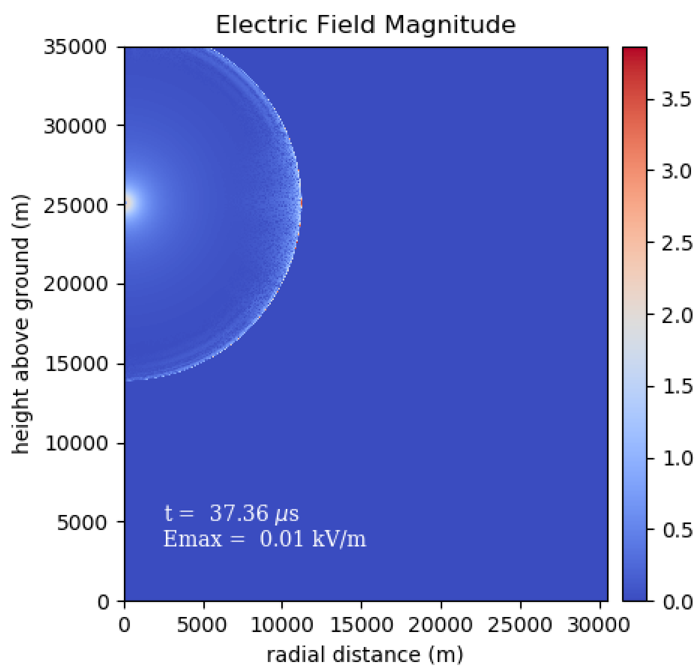

Figure 39: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

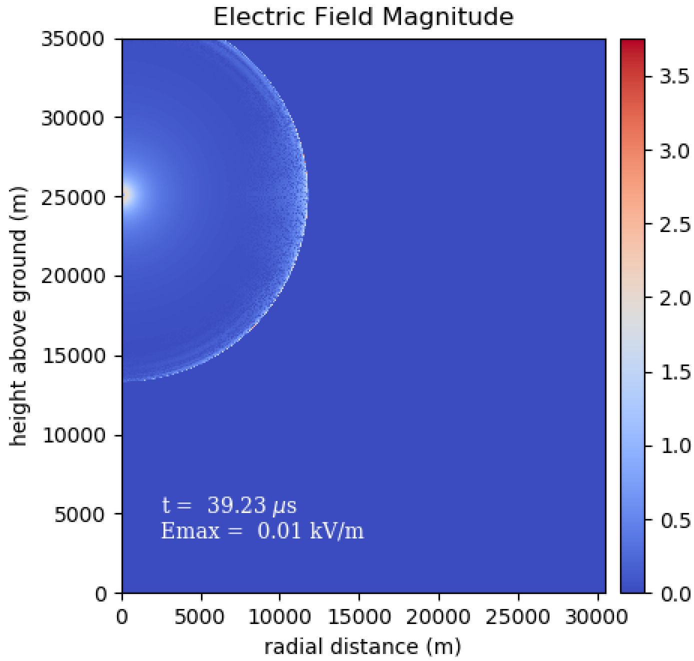

Figure 40: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

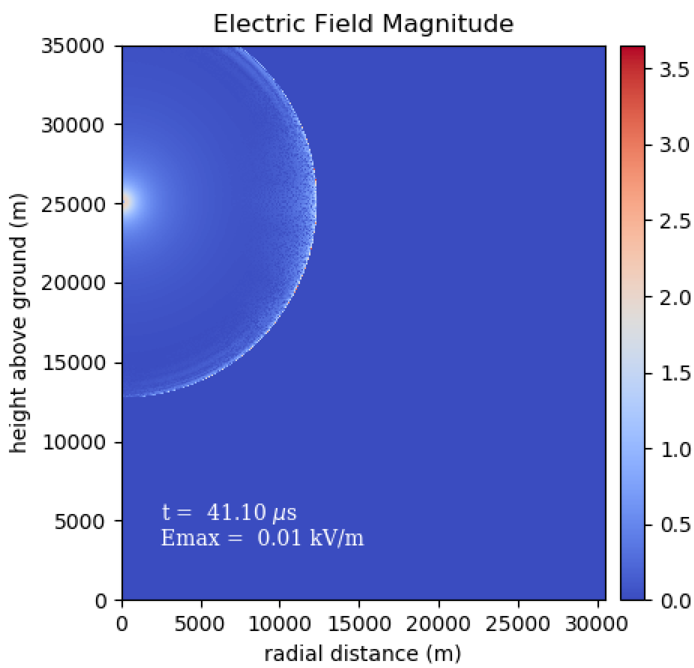

Figure 41: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

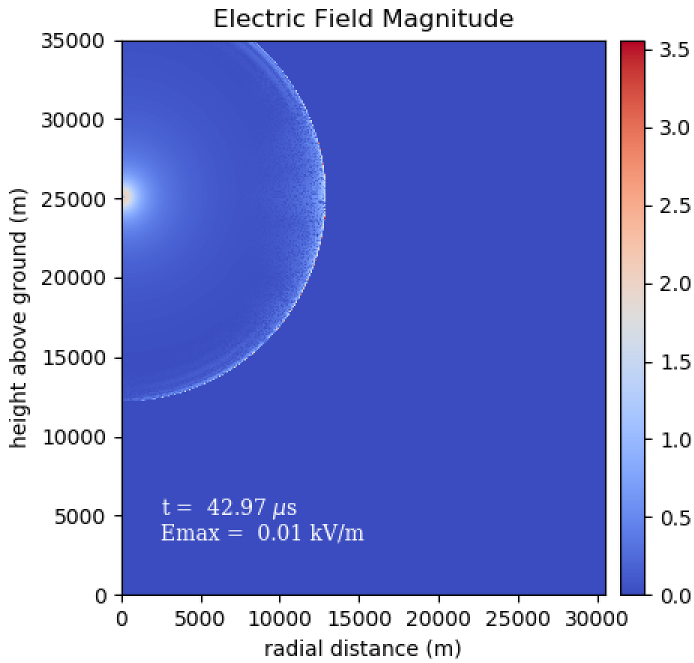

Figure 42: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

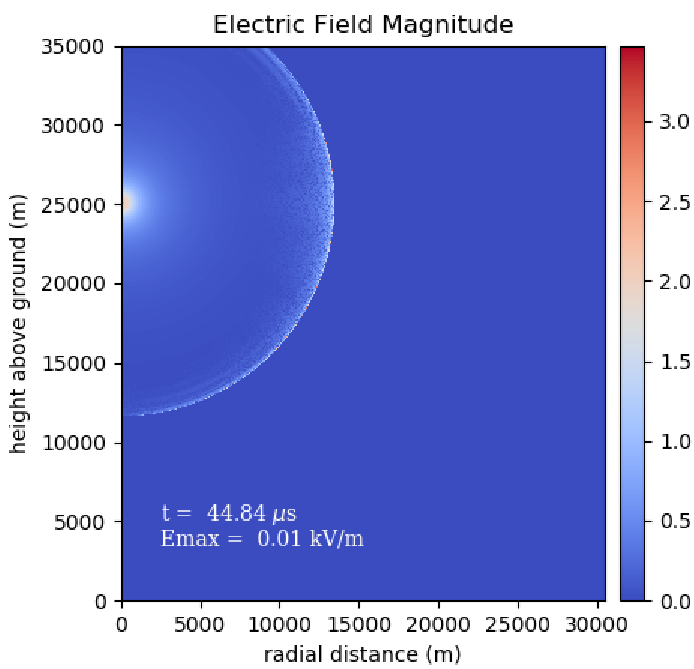

Figure 43: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

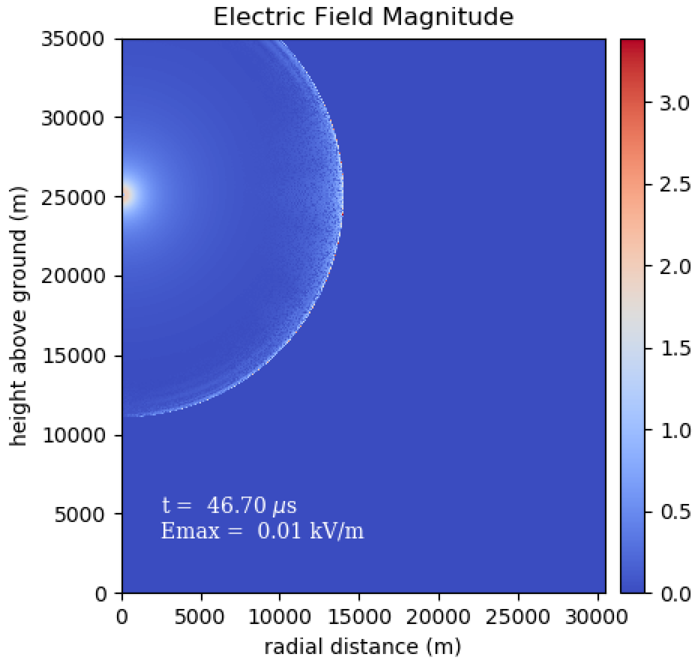

Figure 44: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

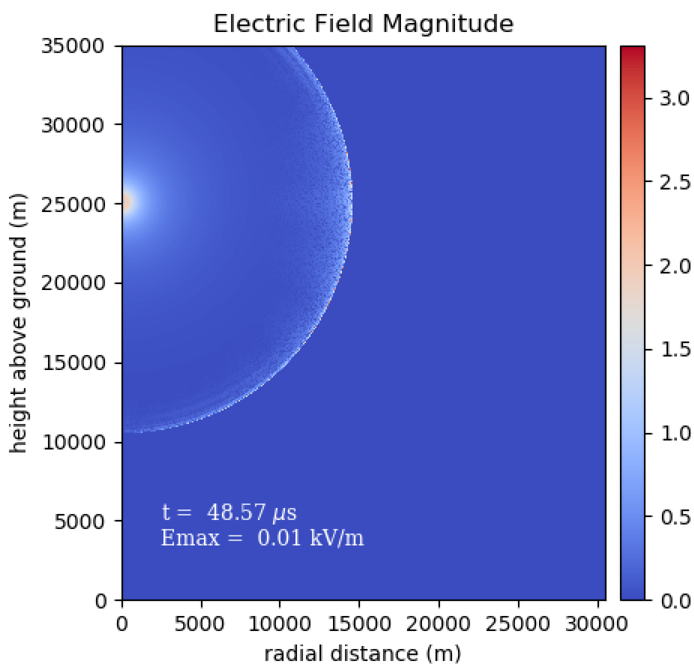

Figure 45: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

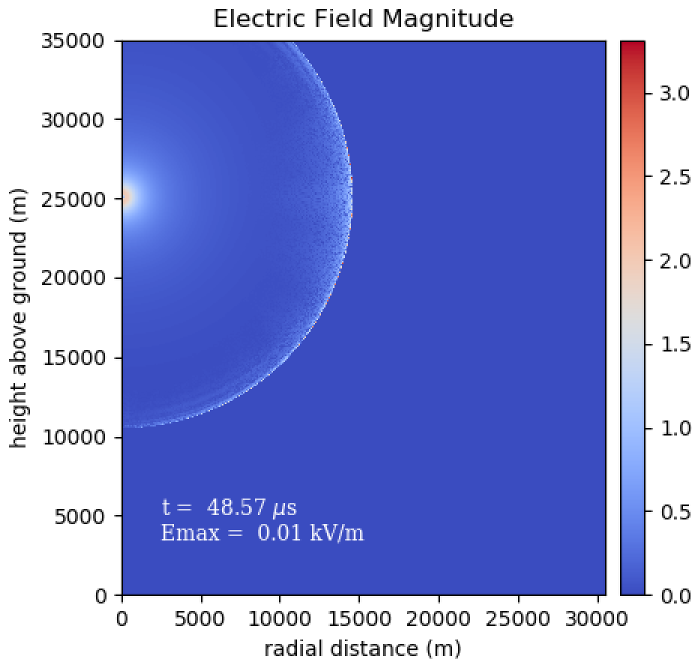

Figure 46: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

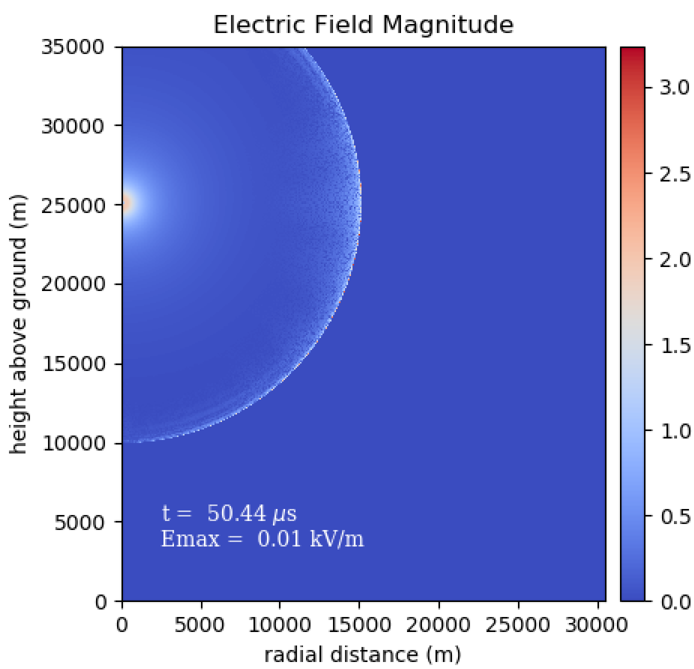

Figure 47: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

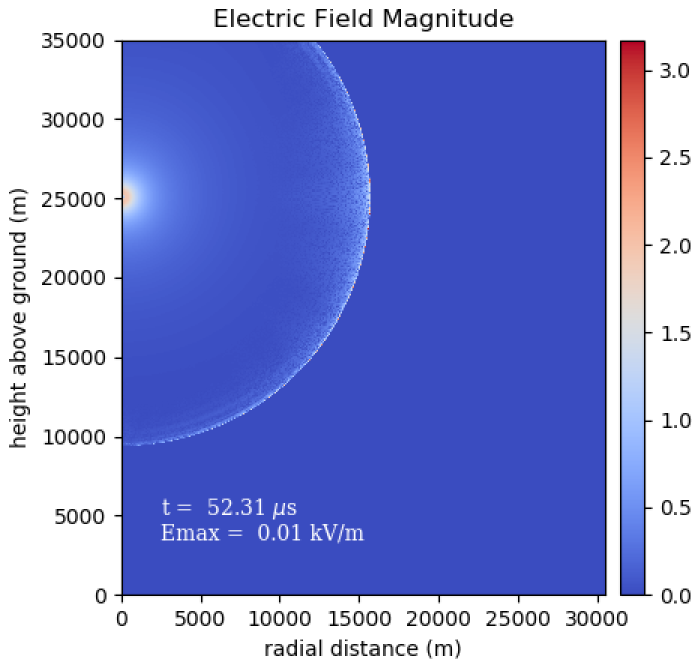

Figure 48: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

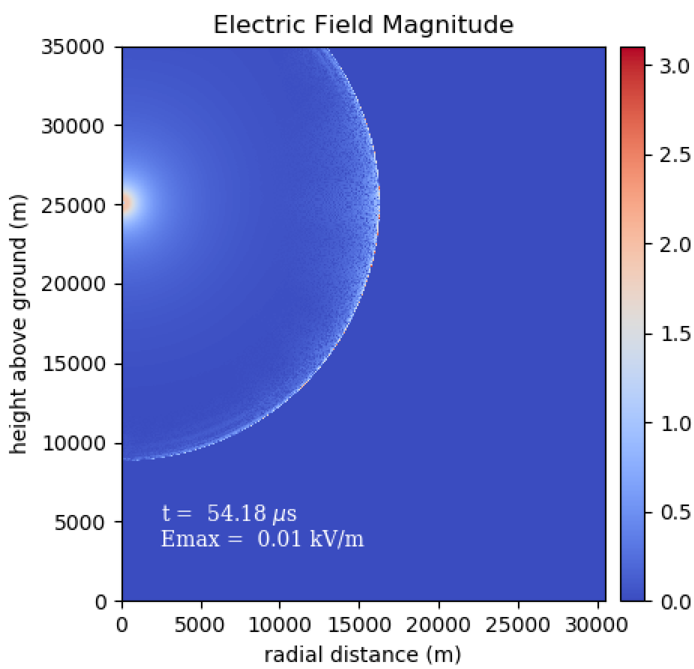

Figure 49: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

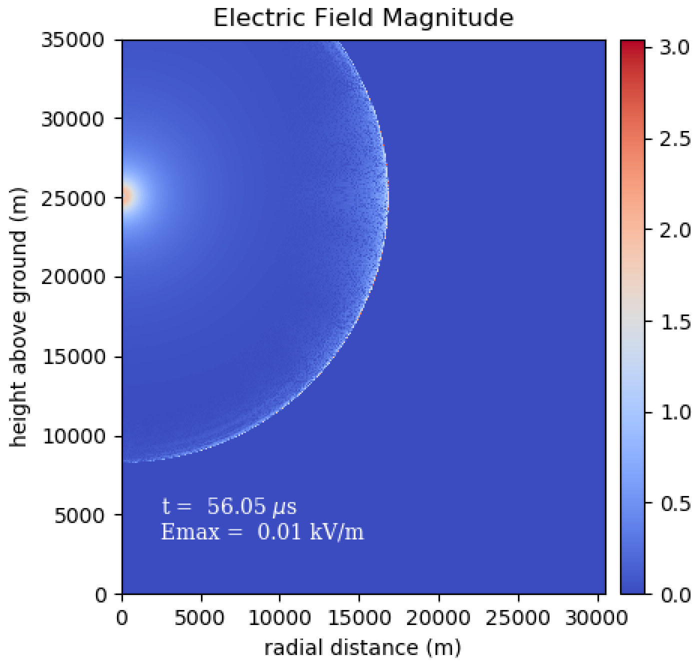

Figure 50: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

4.3 60 km HOB, Artificial MCNP Data

This section contains images from the 60 km ”Art. 3” simulation.

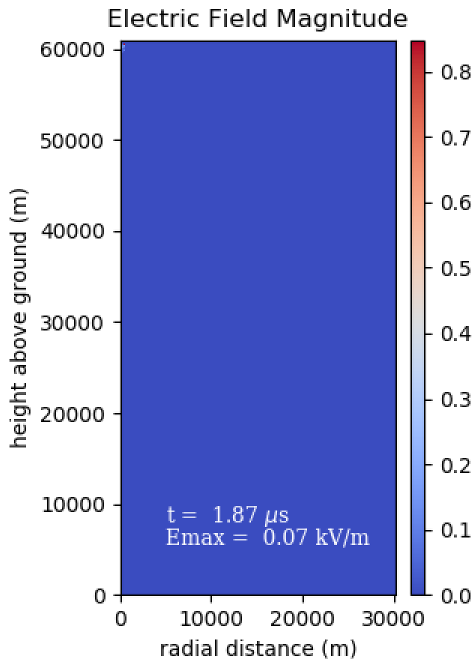

Figure 51: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

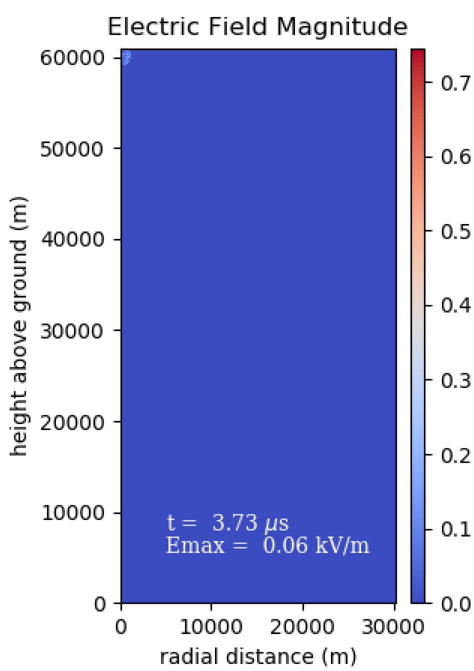

Figure 52: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

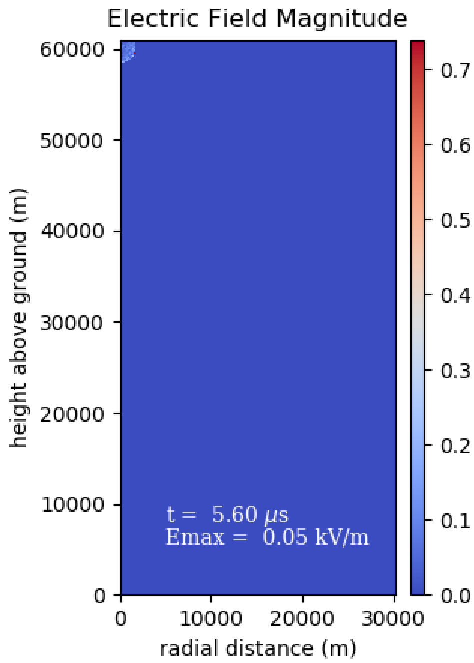

Figure 53: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

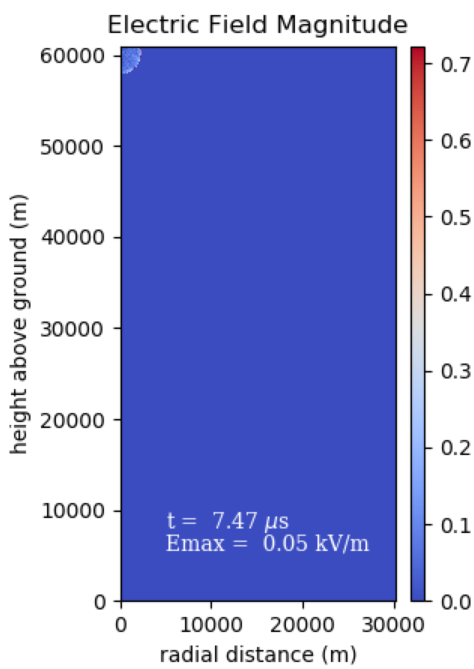

Figure 54: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

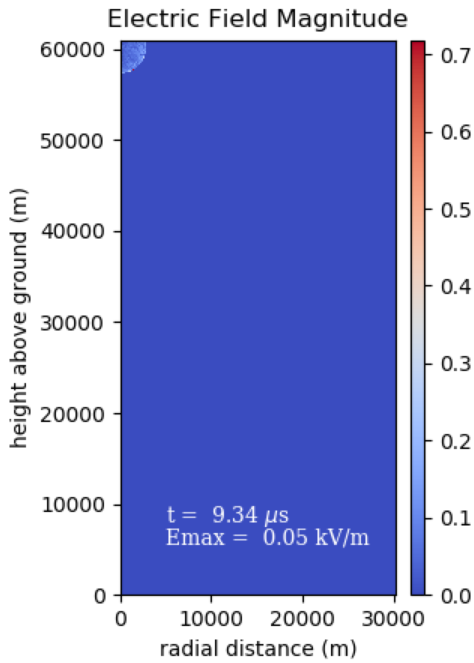

Figure 55: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

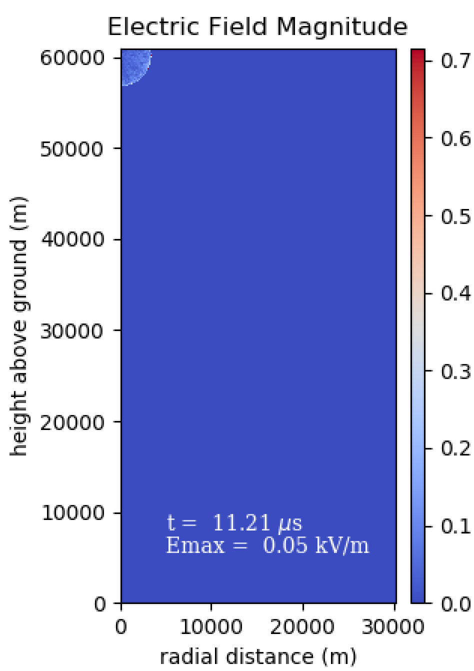

Figure 56: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

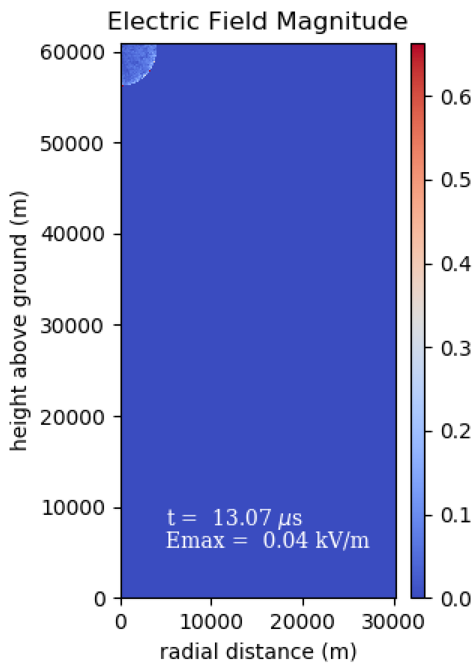

Figure 57: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

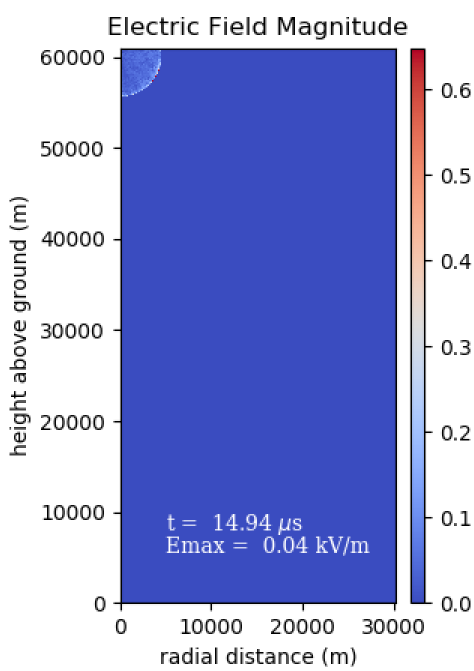

Figure 58: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

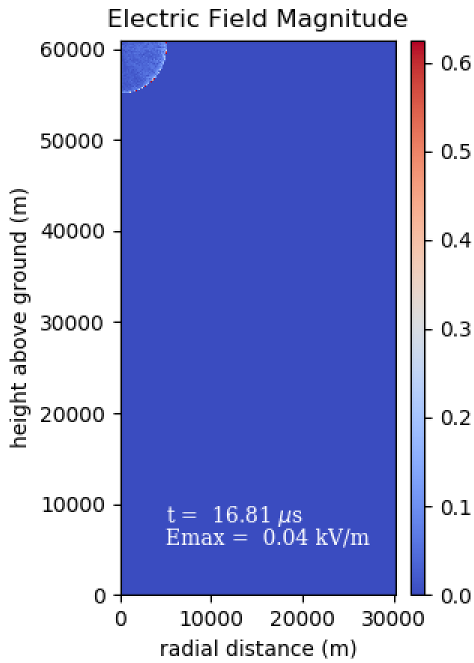

Figure 59: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

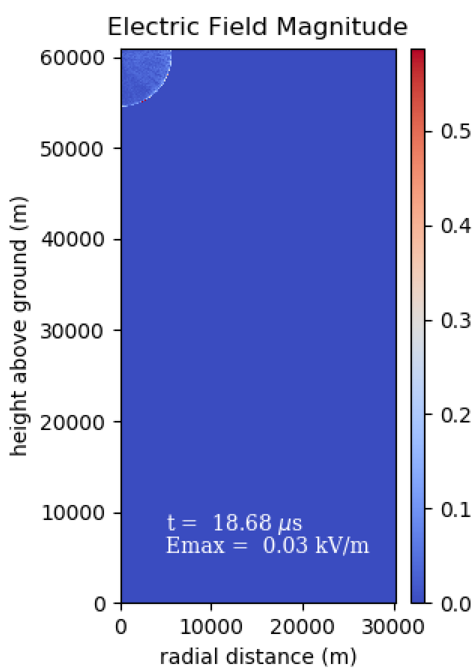

Figure 60: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

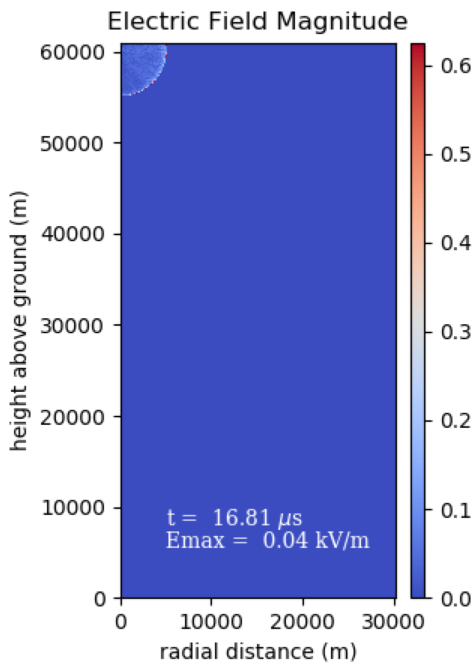

Figure 61: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

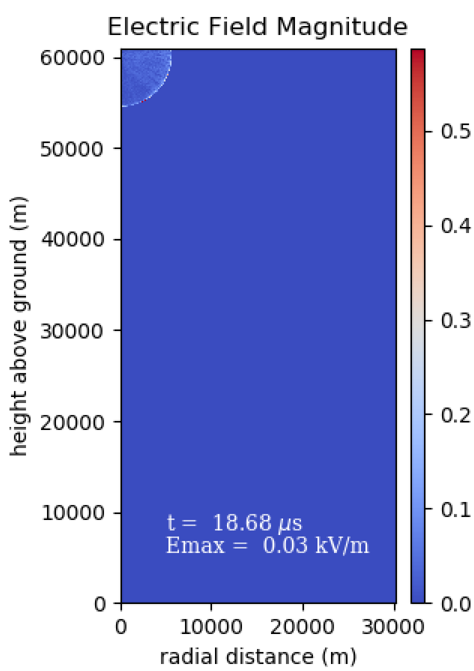

Figure 62: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.

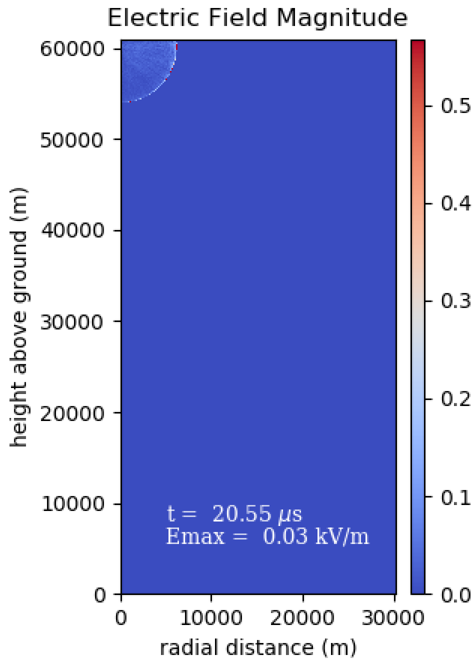

Figure 63: See figure above for time and maximum electric field magnitude. Color scale in figure is in $\sqrt{kV/m}$.