

WebMANTIS and VisualMANTIS Manual Version 1.0

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Chapter 1

INTRODUCTION

This manual contains information on compiling and executing the WebMANTIS and VisualMANTIS graphical interfaces. Both softwares are based on hybridMANTIS (5), a Monte Carlo package for modeling indirect x-ray detectors with columnar scintillators. The application is written in HTML, jQuery, and PHP and can be accessed through a web browser. WebMANTIS is a web based visualization interface that enables the user to control simulation properties through a user interface within a web browser; it can also be accessed through the browsers (such as Mozilla Firefox and Chrome) of mobile devices such as smartphones or tablets. WebMANTIS acts as a server backend and communicates with an NVIDIA GPU computing cluster, therefore it can support a multi-user environment where users can execute different experiments in parallel. The output consists of the point response function (PRF) images, pulse height spectra (PHS) images, and optical transport statistics generated by hybridMANTIS. The users can also download the output images and statistics through a zip file for future reference. In addition, it provides a visualization window that displays a few selected optical photon paths as they get transported through the detector columns and allows the user to trace the history of the optical photons.¹

VisualMANTIS is a simplified single user stand alone version of WebMANTIS that is executed on

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a workstation. These graphical interfaces expand the capability of hybridMANTIS by enabling users to set up their own computational experiments on any GPU computing resource. Although both by defaults utilize the GPUs to accelerate computation time, both can also utilize the CPU if a GPU device is not available. The library dependencies required to build and execute are elaborated in the sections below. The chapters below will instruct the user on the dependencies required to build the application; along with steps for execution and usage. The last chapter provides information on the various aspects of the visualization and how the user can interact with them.

Chapter 2

DISCLAIMER

This software and documentation (the Software) were developed at the Food and Drug Administration (FDA) by employees of the Federal Government in the course of their official duties. Pursuant to Title 17, Section 105 of the United States Code, this work is not subject to copyright protection and is in the public domain. Permission is hereby granted, free of charge, to any person obtaining a copy of the Software, to deal in the Software without restriction, including without limitation the rights to use, copy, modify, merge, publish, distribute, sublicense, or sell copies of the Software or derivatives, and to permit persons to whom the Software is furnished to do so. FDA assumes no responsibility whatsoever for use by other parties of the Software, its source code, documentation or compiled executables, and makes no guarantees, expressed or implied, about its quality, reliability, or any other characteristic. Further, use of this code in no way implies endorsement by the FDA or confers any advantage in regulatory decisions. Although this software can be redistributed and/or modified freely, we ask that any derivative works bear some notice that they are derived from it, and any modified versions bear some notice that they have been modified.

Chapter 3

PREREQUISITES

3.1 Library Dependencies

- Some flavor of Linux e.g. www.ubuntu.com
- hybridMANTIS @ <http://code.google.com/p/hybridmantis/>
- VisualMANTIS
- libevent @ <http://libevent.org/>
- Ubuntu LAMP @ <https://help.ubuntu.com/community/ApacheMySQLPHP>
- CUDA 4.2 or higher, python, gfortran, GNU Scientific Library, gnuplot

WebMANTIS has only been built and tested on Ubuntu 12.04 LTS so far. Both hybridMANTIS and VisualMANTIS are required prior to utilizing WebMANTIS as WebMANTIS is dependent on codes from both, moreover, WebMANTIS also uses the VisualMANTIS executable to start the simulation. The libevent library is required in order to run the backend server that handles communication between the GPU and the graphical front-end. Ubuntu LAMP is required in order to use the current operating system as a webservice such that users can be connected in order to use WebMANTIS. CUDA is required in order to compile and run both hybridMANTIS and VisualMANTIS, detailed instructions for compiling and installing CUDA can be found in the sections below.

Chapter 4

BUILDING HYBRIDMANTIS

WebMANTIS relies on the existing libraries and code that exists in hybridMANTIS, so it is important to have a working implementation of hybridMANTIS ready. The latest version of hybridMANTIS is available for download from <https://code.google.com/p/hybridmantis>. In order to compile and execute hybridMANTIS, additional libraries in the following subsections are required.

4.1 Install gfortran

This library is required because the X-ray and electron transport in hybridMANTIS is performed using PENELOPE (4) which is written in Fortran. On Ubuntu Linux, gfortran can be installed with *sudo apt-get install gfortran*.

4.2 Nvidia CUDA Instructions

There are a wide range of documentation and guides online for installing CUDA on various Ubuntu versions (2)(3)(1) and it is highly suggested the user go through them. It is imperative that the CUDA SDK is installed as hybridMANTIS relies on libraries in the SDK to compile correctly.

4.3 Install GNU Scientific Library (GSL)

On Ubuntu Linux, libgsl can be installed with *sudo apt-get install libgsl0-dev*

4.4 Install GNUPLOT

Gnuplot is required for plotting purposes and can be downloaded using *sudo apt-get install gnuplot*. The visualization was successfully tested with gnuplot 4.6.

4.5 Compile

Once the libraries have been installed and verified, hybridMANTIS can be compiled and executed using the `compile_ver1_0.sh` file. This file contains the script to compile and link the entire program together. Before it can be executed, it must be modified in order to link different libraries, for instance:

- `-I/usr/local/cuda/include`
- `-I/home/user/NVIDIA_GPU_Computing_SDK/C/common/inc`
- `-L/usr/local/cuda/lib64/`
- `-L/home/user/NVIDIA_GPU_Computing_SDK/C/lib`

The libraries above are dynamically linked during compilation and the locations are dependent on the where CUDA and the CUDA SDK are installed.

Chapter 5

BUILDING VISUALMANTIS

VisualMANTIS is a stand-alone application that requires compilation and execution in a Linux-based environment. It relies on similar functions that hybridMANTIS utilizes so therefore it is imperative that hybridMANTIS functions correctly. The following steps are required to merge the functions of hybridMANTIS with VisualMANTIS together.

- Ensure that all libraries in Chapter 4 are working and built correctly.
- Copy all files and folders from `visualMANTIS_v1.0` to the `hybridMANTIS` folder.
- Compile with *`sh compile_visualmantis_ver1_0.sh`*

Chapter 6

BUILDING WEBMANTIS

The following steps details the process of building and executing WebMANTIS. At the end of this chapter, the user should be able to access WebMANTIS through a web browser.

6.1 Install libevent

The event notification library, libevent, is utilized in order to support the multiple user capabilities of WebMANTIS, it utilizes Pthreads to handle multiple connections at once and provides a scalable event notification system for handling large number of users. The library can be downloaded from <http://libevent.org/>, our current implementation has been tested with libevent-2.0.21-stable version. The file contains a README which contains further instructions on compiling and executing in a Linux environment.

6.2 Install Apache LAMP

Apache LAMP is required for WebMANTIS to initialize web service capabilities on a cluster via its public web directory such that it can be accessed by web browsers. The instructions for installing Apache LAMP can be found at <https://help.ubuntu.com/community/ApacheMySQLPHP>. The main libraries needed from Apache LAMP are the Apache webserver and PHP. After installation, you can open up a browser and check the localhost ip address of 192.168.0.1 to ensure it is working correctly.

6.3 Compiling WebMANTIS

After the libevent library has been installed, there is a libevent-thread folder that contains the server code for handling multiple users and it needs to be compiled. This folder can be found in the WebMANTIS folder and run *sh compile.sh* to compile the code.

Copy the WebMANTIS folder to */var/www/* in the Linux directory (it is also possible change this default directory). Write permissions are required for the WebMANTIS folder in order to execute the background PHP and Shellscripts, they can be initialized using the following command: *chmod a+x file1.c file2.c*

Start the libevent server program called *echoserver_threaded*. Open a browser and go to 192.168.0.1 and if WebMANTIS is working correctly, then the graphical interfaces listed in the Chapter 7 below can be seen. Currently, WebMANTIS requires HTML 5 have only been tested to run correctly on Mozilla Firefox and Chrome browsers.

6.4 Web Access

At the moment, WebMANTIS can only be accessed by a browser through the localhost ip address 192.168.0.1 and will work with other users all connected in the local area network. However, in order to give permissions to users outside of the network, please consult the network administrator on opening up the ports for http and giving the cluster an external IP address. Since this topic goes beyond the scope of this work, it won't be elaborated further.

Chapter 7

VISUALIZATION

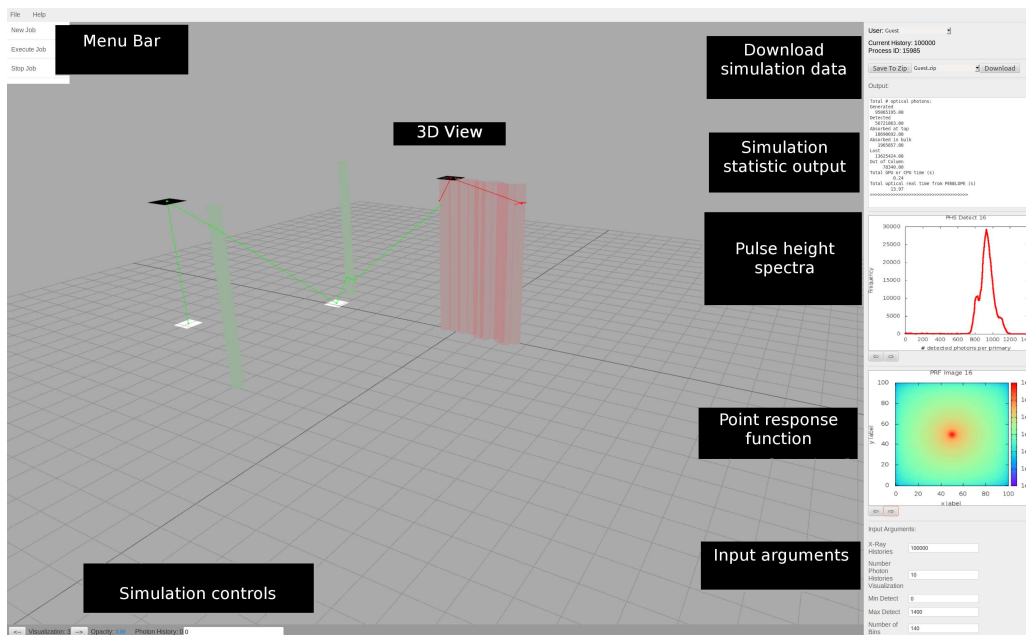


FIG. 7.1. Shows the different sub-sections of the WebMANTIS visualization. There are eight sub-sections that make up WebMANTIS: **Input Arguments**, **Menu**, **3D View**, **Simulation Controls**, **Download Simulation Data**, **Simulation Statistic Output**, **Pulse Height Spectra**, **Point Response Function**. The figure illustrates cylinders marked in red with some degree of transparency and it is possible to see optical photon trajectories as indicated by the red and green lines. The black box represents the top surface of the material while the white box marks the bottom surface. Optical photons can either get reflected or absorbed when hitting these surfaces.

7.1 Input Arguments

This section allows the user to change the input simulation parameters. Parameters are same as the parameters described in hybridMANTIS (more information is listed in the hybridMANTIS manual), except one new parameter **Number Photon Histories Visualization** which indicates the number of photon histories to save out of the initial 100000 histories specified by x-ray histories. A full list of all possible input arguments is also provided in Figure 7.2 below.

The following list contains the input parameters name along with a detailed description.

- **X-Ray Histories** : number of x-ray histories to be simulated (N)
- **Min Detect** : min. number of optical photons that can be detected
- **Max Detect** : max. (mean energy of input spectra * yield) number of optical photons that can be detected
- **Number of Bins** : number of bins for storing pulse height spectrum (maximum value=1000)
- **X-Dimension** : length of scintillator (in microns)
- **Y-Dimension** : width of scintillator (in microns)
- **Detector Thickness** : thickness of detector (in microns), hybridMANTIS assumes the center of z dimension to be at 0 and (min, max) being (-thickness / 2, thickness / 2)
- **Column Radius** : radius of a column in the scintillator (in microns)
- **Column Refractive Index** : refractive index of column material (default is CsI with refractive index of 1.8)
- **Inter-Columnar Refractive Index** : refractive index of inter-columnar material (default is Air with refractive index of 1.0)

- **Top Surface Absorption Fraction** : absorption fraction at the top surface of the scintillator
- **Bulk Absorption Coefficient** : absorption coefficient in the bulk of the columns (in 1/microns)
- **Surface Roughness Coefficient** : determines the degree of roughness in the column walls
- **Minimum Distance Next Column** : minimum distance to the next column based on columnar crosstalk (in microns)
- **Maximum Distance Next Column** : maximum distance to the next column based on columnar crosstalk (in microns). The distance to next column is sampled uniformly between min and max distances.
- **PRF Image X Lower Bound** : x lower bound of PRF image
- **PRF Image Y Lower Bound** : y lower bound of PRF image
- **PRF Image X Upper Bound** : x upper bound of PRF image
- **PRF Image Y Upper Bound** : y upper bound of PRF image
- **Light Yield** : scintillator light yield (/eV)
- **Pixel Pitch** : pixel pitch (in microns) (max. pixels allowed in PRF image are 501x501. calculate this by (upper bound - lower bound)/pixel pitch.)
- **Non-Ideal Sensor Reflectivity** : reflectivity of non-ideal sensor plane (between 0 and 1)
- **GPU (1) or CPU (0) flag** : flag for running in the GPU + CPU (1) or only in the CPU (0)
- **Machine Number** : this is helpful when running several simulations with exactly same optical parameters; the output file names contain the optical parameters with machine number appended at the end of file name.

- **Number Photon Histories Visualization** : number of photon histories to save for visualization (e.g. 10, this means that the first ten optical photons simulated by hybridMANTIS is retrieved from the GPU for visualization and the user can modify this variable to visualize more histories; the only caveat being the amount of memory required to save the data)

7.2 Menu

After making changes in the **Input Arguments** window, clicking **Execute Job** will start executing the visualization code of hybridMANTIS and show the visualizations in the the main **3D View** window. This section also provides a **Stop Job** button that allows the user to stop their current executing job which instantly kills the job without dumping any log files and frees up the computational resources in the cluster.

7.3 Simulation Statistic Output

Figure 7.3 shows the direct output of webMANTIS during execution and is useful as a guideline in the simulation time-line.

7.4 3-Dimensional View

The 3D window shows all of the photon histories. It allows the user to interact with it through the use of a mouse in rotating and zooming in regions of interest. The different colored cylinders indicate that the current photon has interacted with it. As a photon can potentially hit the ceiling and floor and perish, it is plausible for the CUDA kernels to generate a new photon that start another process of interacting with the materials. These different colored cylinders represent that. The top ceiling is also represented via a black square box while the bottom surface is represented as a white square block. Optical photons hitting these the top and bottom surface will reflect back into the material depending on their trajectory or they might get absorbed or detected.

Input Arguments:	
X-Ray Histories	100000
Number Photon Histories Visualization	10
Min Detect	0
Max Detect	1400
Number of Bins	140
X-Dimension	909
Y-Dimension	909
Detector Thickness	150
Column Radius	5.1
Column Refractive Index	1.8
Inter-Columnar Refractive Index	1
Top Surface Absorption Fraction	0.1
Bulk Absorption Coefficient	0.0001
Surface Roughness Coefficient	0.2
Minimum Distance Next Column	200
Maximum Distance Next Column	280
PRF Image X Lower Bound	0
PRF Image Y Lower Bound	0
PRF Image X Upper Bound	909
PRF Image Y Upper Bound	909
Light Yield	0.055
Pixel Pitch	9
Non-Ideal Sensor Reflectivity	0.25
Machine Number	1

Output:

```
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
OPTICAL TRANSPORT STATISTICS

!! Simulation in the GPU !!

Total # optical photons:
Generated
95065195.00
Detected
55727030.00
Absorbed at top
8646519.00
Absorbed in bulk
1269665.00
Lost
17391828.00
Out of Column
47134.00
Total GPU or CPU time (s)
0.18
Total optical real time from PENELOPE (s)
11.03
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>

>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
report: SIMULATION ENDED
Results have been written to the corresponding DAT files.
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>

Last random seeds:
330756190 114074384
Elapsed real time (s), excluding init:
1.65484E+02
Elapsed CPU time (s), excluding init:
1.64542E+02
Each report update took (in CPU s):
1.60065E-02
No. of histories simulated:
100000.
CPU Speed (histories/s):
6.07806E+02
CPU Speed without load balancing time (histories/s):
6.30810E+02
```

FIG. 7.3. Output data

FIG. 7.2. Input arguments

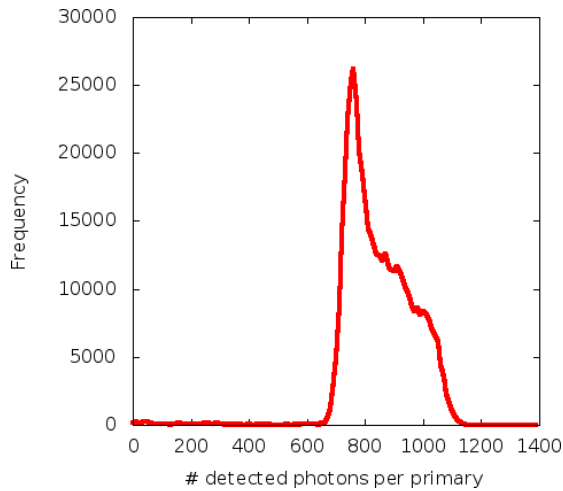


FIG. 7.4. Pulse Height Spectrum

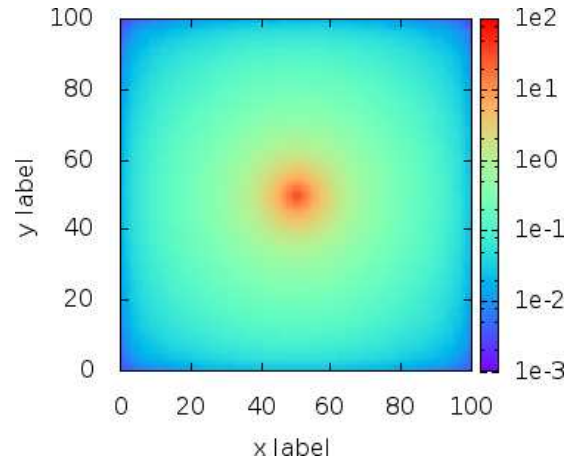


FIG. 7.5. Point Response Image

7.5 Simulation Controls

The **Simulation Controls** allows the user to follow the optical photon trajectories through a sliding bar in a step-by-step fashion. In addition, the user can alter the transparency and view different optical photon histories.

7.6 Pulse Height Spectrum and Point Response Function

Figures 7.4 and 7.5 shows the resulting **Pulse Height Spectrum** and **Point Response Function** images generated by WebMANTIS using **GNUPLOT**.

7.7 Download Simulation Data

This section allows the user to download simulation data and statistics from prior executions via a zip file. The prior simulation data includes optical transport statistics, PRF and PHS output images.

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