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FullMonte: Fast Monte Carlo Light Simulator

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ABSTRACT

Determining the light propagation in heterogeneous media is a challenging task which can only be approximated by solving the Boltzmann transport equation via diffusion theory. However, diffusion theory becomes very inaccurate at interfaces, boundaries, sources, and sinks, which are present in heterogeneous media. Monte Carlo methods are able to converge to the correct solution by simulating a sufficiently high number of photons, at the cost of increased runtime. Therefore, it is important to optimize the Monte Carlo simulator, thereby allowing more photons to be simulated and a more accurate solution within a given runtime. FullMonte is a full-featured simulator that uses processor-optimized operations to achieve the highest performance of any 3D tetrahedral Monte Carlo light propagation software to date. This paper presents two medical use cases which benefit from FullMonte, highlights new features and explains the optimizations that lead to its high performance.

Keywords: FullMonte, PDT, BLI, Simulator, Monte Carlo

1. INTRODUCTION

When determining light propagation in any kind of media, the Boltzmann transport equation (BTE) needs to be solved. Solving the BTE analytically is possible in some cases, as shown by Gressmann and Strain,[1] but applying these solutions to complex geometries is generally not possible. For these problems, diffusion theory provides an analytic solution to the Boltzmann transport equation but it is error prone at media interfaces and boundaries and at photon sources and sinks.[2] In contrast, numerical methods, such as Monte Carlo (MC) methods, converge to the correct solution when a sufficiently high number of particles are simulated. MC methods have been used successfully to calculate light propagation in 2D layered media,[3] and 3D media represented by voxel[4] or tetrahedral meshes.[5] The accuracy of MC methods improves with the number of simulated particles at the expense of runtime. Consequently, a trade-off must be made between the simulation's accuracy and runtime, motivating a fast light propagation simulator. This challenge led to the development of FullMonte, a MC-based light propagation simulator which outperforms all other available simulators of its kind.[6]

In Section 2, this paper presents two medical research use cases where FullMonte is being employed. Sections 3 and 4 introduce new features and performance enhancements of FullMonte. Section 5 concludes this paper.

2. FULLMONTE USE CASES AND WORKFLOW

FullMonte supports workflows for both photodynamic therapy (PDT) and bioluminescent imaging (BLI).The challenge in PDT is to determine the best light source placement and energy intensity in order to destroy a sufficient amount of the diseased cells, i.e. a cancerous tumor or a bacteria infection, while minimizing the damage to the surrounding healthy tissue.[7] With a simulator to predict the outcome of a planned treatment, the medical team can determine the best possible source placement and energy intensity beforehand in order to apply the treatment with the highest success rate.

In BLI, some cells of the subject's body are modified to emit light.[8] The light emitted from the subject's body is then measured to localize the origin of the light emitting tissue. Currently, BLI is used in laboratory research to track the size and location of cancerous tumors. The main challenge is developing a methodology to solve the optical inversion problem, for which a fast light simulator is a key tool.

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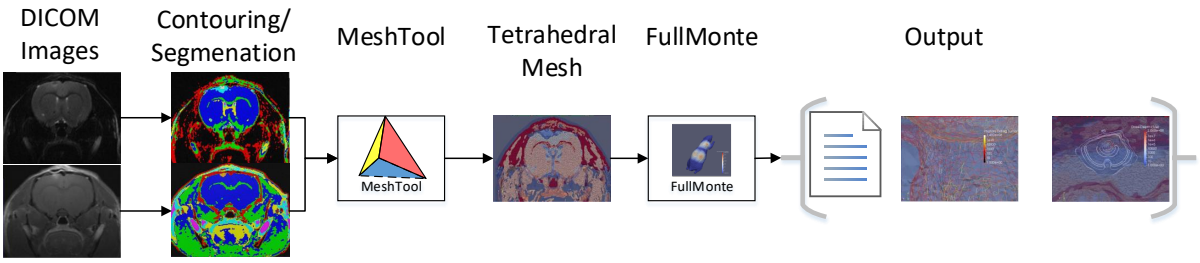

Figure 1. FullMonte workflow starting from clinical images and ending at various output options.

FullMonte for PDT treatment planning is only as effective as the quality of the diagnostic radiology that produces the patient-specific tissue structure and geometry that is input to FullMonte. To support FullMonte-based treatment planning we have designed the workflow illustrated in Figure 1 which allows the use of standard *DICOM* clinical images, contouring of the relevant organs and structures, and the generation of high resolution in-silico models. The contouring information of the clinical images serves as input to a meshing software called MeshTool to create a 3D tetrahedral mesh which can be used by FullMonte. This allows FullMonte to output both a new VTK mesh with annotated fluence or absorbed energy values, or just the fluence values associated with each tetrahedron of the input mesh. Given the energy absorbed in each tetrahedron, post-processing TCL commands compute the PDT dose throughout the tissue. For the BLI use case, the fluence values of interest are those on the exterior surface triangles as those represent the light exiting/detected; FullMonte can also output a mesh containing only the exterior surface triangles of the original tetrahedral mesh to simplify BLI analysis.

3. FULLMONTE FEATURES

FullMonte has been developed for medical professionals. It is written in highly optimized C++ code, but has been fully integrated with the TCL scripting language with example flows that can be used as is or extended to meet the specific needs of users. Using the TCL interface, customized simulation runs and outputs can be created using FullMonte, without the challenge of modifying complex C++ code. FullMonte outputs *Visualization Toolkit* (VTK) formatted meshes which allows them to be viewed using popular open-source tools like *Paraview*. Commonly logged statistics, such as volume absorption and surface interface events, are predefined in FullMonte and exposed through the TCL interface.

FullMonte light sources launch *packets* of photons by assigning them a position and direction in 3D space based on the source's attributes. The most basic light source is an `Isotropic Point` which emits light uniformly in all directions from a single point. Support for more advanced light sources has been developed based on input from our medical partners. For example, the `Line`, `PencilBeam`, and `Cutend Fiber` are used primarily in PDT, while the `Ball` and `Tetrahedral Volume` are used primarily in BLI. Multiple sources can be grouped together by using the `Composite` source. In this case, each source within the `Composite` is given a relative *intensity* to control the percentage of packets that it emits.

FullMonte uses the *Fast Mersenne Twister* by Saito and Matsumoto[9] to efficiently generate high quality random numbers. The random number generator is *pseudorandom* which means that, given the same initial *seed*, successive simulations will produce identical results. Therefore, changes in the treatment simulation can be more easily investigated without needing to consider the additional variance from differences in the random numbers. This gives the user of FullMonte more control over the behaviour of the simulation.

4. COMPUTATIONAL EFFICIENCY

The accuracy of a MC method depends on the number of particles it is able to calculate in a *reasonable* time. The higher that number is, the more accurate the results will be. Therefore, it is extremely important to improve the performance of a MC method as much as possible to enable more statistically accurate simulations. We have gathered measurements on a machine running an 8-core 3.5 GHz Intel Xeon CPU with 64 GByte RAM. The installed OS is Ubuntu 16.04 LTS which is recommended for running FullMonte. The simulation uses a mesh of a human jaw and neck with 1088680 tetrahedrons and the number of photons simulated is 10^6.

Table 1. Computational performance of FullMonte at different optimization levels

Optimization Level	Runtime (sec)	Speedup
Generic Single-Thread (**Baseline**)	316	–
Generic Multi-Thread (8 threads)	54	6x
AVX Code Single-Thread	39	8x
AVX Code Multi-Thread (8 threads)	9	34x
AVX2 Code Multi-Thread (8 threads)	8	**36x**

As shown in Table 1, using 8 threads yields a 6x speed-up over the generic code. FullMonte goes further, and uses processor-optimized operations called AVX/AVX2 instructions (which work on short vectors of numbers at once) to achieve an 8x improvement. Combining these optimizations yields a performance gain of 36x over the baseline and makes FullMonte the fastest available 3D tetrahedral MC light simulator.[6]

FullMonte is memory efficient. The memory required depends on the number of tetrahedrons in the simulation mesh; moderate size geometries (10^6 tetrahedrons) require less than 1 GB, while large meshes (10^7) require approximately 5 GB. The number of threads does not influence the memory usage since all threads access the same mesh. Since each thread does not require its own copy of the mesh, the total memory usage is reduced.

Based on the performance and memory results we can give a recommendation for a system to run FullMonte. The processor can be either an AMD or Intel processor manufactured in 2013 or later to ensure it supports at least the AVX operations. The memory requirement is highly dependent on the size of the meshes the user wants to simulate, but 16 GB is generally ample.

5. CONCLUSION

FullMonte is the fastest 3D tetrahedral MC light simulator to date. Its workflow enables more general PDT treatment planning, helping make PDT a more widely applicable cancer treatment. In the past, PDT was only feasible in restricted cases where the outcome could be predicted by experience or simpler simulators. FullMonte fills this void by allowing treatments to be simulated and optimized prior to administration. We are enhancing FullMonte with new features to accommodate the simulation and workflow needs of medical professionals in PDT and other domains while exploring methods to further improve the performance of the simulator.

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