IMPLEMENTATION OF THE FINITE-DIFFERENCE TIME-DOMAIN METHOD USING GRAPHICS PROCESSING UNITS

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IMPLEMENTATION OF THE FINITE-DIFFERENCE TIME-DOMAIN METHOD USING GRAPHICS PROCESSING UNITS

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I thank my committee for their patience, insight and unfailing encouragement. Without them, this thesis would remain vaporware. Never give up, never surrender!

Lively , S. David B.S.E.E, Southern Methodist University, 2008

Implementation of the Finite-Difference Time-Domain Method Using Graphics Processing Units

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Traditionally, optical circuit design is tested and validated using software which implement numerical modeling techniques such as Beam Propagation, Finite Element Analysis and FDTD.

While effective and accurate, FDTD simulations require significant computational power. Existing installations may distribute the computational requirements across large clusters of high-powered servers. This approach entails significant expense in terms of hardware, staffing and software support which may be prohibitive for some research facilities and private-sector engineering firms.

Application of modern programmable GPGPUs to problems in scientific visualization and computation has facilitated dramatically accelerated development cycles for a variety of industry segments including large dataset visualization, microprocessor design, aerospace and electromagnetic wave propagation in the context of optical circuit design.

The FDTD algorithm as envisioned by its creators maps well to the massively-multithreaded data-parallel nature of GPUs. This thesis explores a GPU FDTD implementation and details performance gains, limitations of the GPU approach, optimization techniques and potential future enhancements that may provide even greater benefits from this underutilized and often-overlooked tool.

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To Audrey, Wyatt, Walter and Gwendolyn

Chapter 1

Introduction

The FDTD [1] algorithm is the underlying mechanism used by many commercial RF simulation packages, as well as open source software such as MIT's Meep.

Given the computationally-intensive nature of FDTD, organizations requiring simulation of large domains or complex circuits must provide significant resources. These may take the form of leased server time or utilization of an on-site high-performance cluster, amongst other options.

In this thesis, we explore an implementation of FDTD utilizing graphics processing units (GPUs). Initially designed to perform image generation tasks such as those required by games, cinema and related fields, modern versions are well-suited for general computation work. GPUs are now enjoying wide adoption in fields such as machine learning and artificial intelligence, medical research, signals analysis and other areas which require rapid analysis of large datasets.

Even modern consumer-grade GPUs offer thousands or tens of thousands of processing units (”cores”), while high-end CPUs typically offer 4-8 cores. While the two are not interchangeable, some algorithms, such as FDTD, require little or no data interdependence, no branching logic (a severe performance impediment on GPUs) and consist of short cycles of simple operations. The power of the GPU lies in performing these simple operations at large scale, with thousands of threads running in parallel.

The following sections detail FDTD. Later sections describe a CPU-based implementation (MIT's Meep simulator), and our GPU-based GoLightly simulator. We verify the GPU solution numerically, and compare performance between CPU- and

GPU-based implementations. Finally, we consider future applications and enhancements.

1.1. FDTD Overview

At it's heart, FDTD expresses Maxwell's equations as a discretized set of time-domain equations. These equations describe each electric field component in terms if its orthogonal, coupled magnetic fields, and each magnetic field component as a function of its coupled, orthogonal electric fields.

1.1.1. Wave equation

In a TM_z time domain simulation, wave equation for E_z is of the form:

$$\frac{\partial E_z}{\partial t} = K * (\frac{\partial H_x}{\partial y} + \frac{\partial H_y}{\partial x}) \tag{1.1}$$

Equation 1.1 states that the temporal derivative (change in amplitude) of E_z is a function of the Y-axis spatial derivative of the H_x field and the X-axis spatial derivative of the H_y field.

In order to apply this equation to a computational domain, FDTD defines a cell-based discretization strategy.

1.1.2. Yee Cell

Yee [1] defines a computational unit known as a "cell." The cell describes how each field component within a domain is related to it's coupled fields. For instance, in a 2D TM_z simulation, E_Z depends on adjacent H_y and H_x components. The cell format used in such a simulation is of the form shown in 1.1.

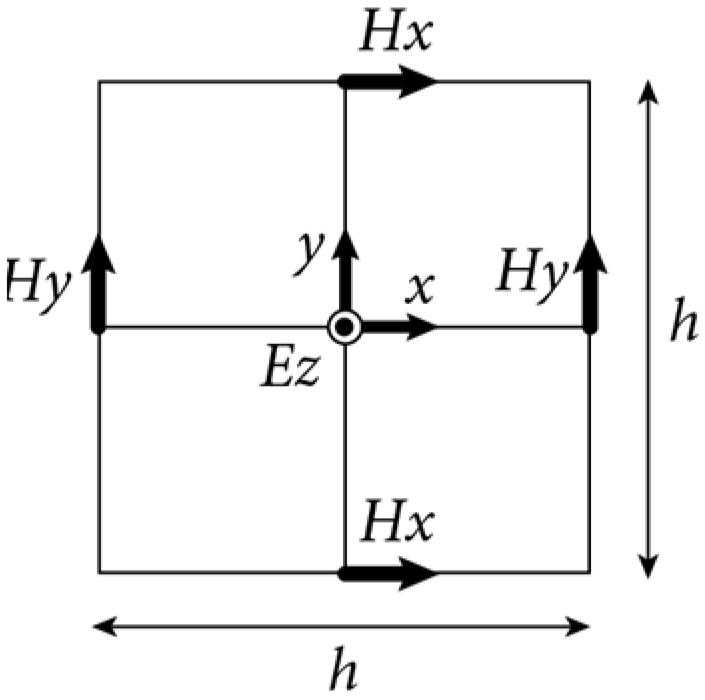

Figure 1.1. 2D TM_Z Yee Cell

More formally, we may expand the E_Z wave equation, arriving at:

$$E_{z i,j}^{\,t} = C_a * E_{z i,j}^{\,t-1} + C_b * (H_{x_{i,j+\frac{1}{2}}}^{t-\frac{1}{2}} - H_{x_{i,j-\frac{1}{2}}}^{t-\frac{1}{2}}) + C_b * (H_{y_{i+\frac{1}{2},j}}^{t-\frac{1}{2}} - H_x y_{i-\frac{1}{2},j}^{t-\frac{1}{2}}) \tag{1.2}$$

Similarly, the equations for the coupled fields H_x and H_y may be expressed as:

$$H_{x i,j}^{\,t} = D_a * H_{x i,j}^{\,t-1} + D_b * (E_{z_{i,j+\frac{1}{2}}}^{t-\frac{1}{2}} - E_{z_{i,j-\frac{1}{2}}}^{t-\frac{1}{2}}) \tag{1.3}$$

$$H_{y_{i,j}}^{\,t} = D_a * H_{y_{i,j}}^{\,t-1} + D_b * (E_{z_{i+\frac{1}{2},j}}^{t-\frac{1}{2}} - E_{z_{i-\frac{1}{2},j}}^{t-\frac{1}{2}}) \tag{1.4}$$

Chapter 2

Device Architecture

CPUs and GPUs each offer advantages for different computational tasks. Multi-core CPUs offer complete, semi-independent cores which are effectively discrete processsors. GPUs, however, offer large-scale parallelization, but require strong data and code coherence in order to achieve acceptable performance.

2.1. CPU

Users typically run many different applications in parallel: a web browser, music player, word processor and email client are a common combination.

In a modern multi-core CPU, each core provides a dedicated ALU and register set. This allows each core to operate as an independent device. This architecture is advantageous when the device is required to perform disparate operations.

However, this approach also introduces some performance limitations. If we wish to perform identical operations on large datasets, we are limited to 4-8 threads. The same processor that excels at executing many different tasks at the same time performs sub-optimally.

When running FDTD on a CPU, each core's ALU executes essentially the same operations on a dedicated register set. Each ALU performs the same operation at the same time, indicating that the additional ALUs are redundant. Thus, the flexible, general-purpose nature of a CPU becomes a liability.

2.2. GPU

GPUs were initially designed for one thing: to determine, as quickly as possibly, what color a pixel should be.

.... more history stuff here...

2.2.1. SIMD

GPUs implement what is known as a single-instruction (SIMD), multiple-data processing model.

In a SIMD architecture, a core may consist of a single ALU, with multiple register banks. Separate "threads" load different data into dedicated register banks. The ALU executes identitical operations on all registers simultaneously.

The approach provides some benefits and limitations:

- Fewer components are required per core since fewer ALUs are required. Leads to reduced die space requirements.
- Better code caching. A single ALU, and corresponding cache, are used for many threads, eliminating the need to load or monitor cache behavior per thread.
- TODO

2.2.2. FDTD in SIMD

TODO: why FDTD maps well to GPUs

Chapter 3

Meep

Meep is a full-featured, open-source simulator produced by the Massachusetts Institute of Technology. In addition to its core FDTD-based simulation engine, it provides a scripting interface for defining models and simulation parameters, recording results, and other tasks.

3.1. Modeling

One limitation of Meep is it's use of an obscure, uncommon scripting language, SCHEME. Models are defined in terms of constructive solid geometry (CSG) commands, whereby the user describes their model in terms of boolean operations and regular polyhedra.

While adequate for simple models, constructing an arbitrarily-shaped or dynamic structure in this way may be difficult. In practice, proprietary software may be used to convert more complex model definitions created in other software into a format usable by Meep.

It is worth noting that Meep provides a "material function" capability. This allows the user to dynamically determine the material properties of a point in space using their own algorithm rather than defining their model using CSG. However, to advantage of this capability, the user must employ additional software or custom programming, further increasing the complexity of an already complicated system.

3.2. Performance

Meep is a mature, highly-optimized suite of tools. While complex to configure and use, it scales well across multiple machines, relying on the MPI protocol to keep nodes within a simulation cluster in sync.

While performant when compared to other FDTD software, Meep suffers from the same architecture-imposed limitations of all CPU-based implementations. The limited number of processing cores available on a general-purpose CPU restricts the number of data points that can be be processed within a given time frame. This problem can be solved by provisioning additional computers which would run in parallel, distributing the computational load evenly across the resulting cluster.

This sort of cluster configuration incurs its own overhead. Although a domain may be divided into chunks and distributed across cluster nodes, FDTD boundary conditions require that, at some point, parts of the divided domain must be exchanged between nodes to maintain continuity. This necessitates installation of a high-speed local network and supporting hardware.

3.3. Limitations

The manner in which models are defined, poor performance on single machines and laptops, incompatibility with Microsoft Windows all indicate that this system is not suitable for rapid design iteration. To that end, we present an alternative, GPU-based approach. (See chapter 4)

Chapter 4
GoLightly

GoLightly is the GPU-based FDTD simulator application that is the focus and product of this thesis. Written using a combination of C++, CUDA and OpenGL, it provides a lightweight yet complete FDTD solution.

4.1. Goals

GoLightly is intended to address deficiencies common to CPU-based solutions. In particular, it is designed to be fast, friendly and portable.

- Fast. An iterative design process requires rapid feedback from the simulator. Long simulation times necessitated by existing solutions inhibit this process.
- Friendly. Definition of models and other simulation parameters should not require expertise in software development or quasi-proprietary scripting languages.
- Portable. Ideally, the simulator should run on a high-end consumer grade laptop and support the most common desktop operating systems (Microsoft Windows and Apple OS X).

To meet those goals, GoLightly takes advantage of the oft-underutilized programmable GPU available in common desktop and laptop computers, resulting in a dramatic speedup. Rather than relying on a proprietary model definition language or obscure, limited scripting system, we use industry-standard image and geometry file formats so that models may be defined using robust, familiar, readily-available tools. By building the software specifically for Microsoft Windows, we ensure that it is compatible with the most common desktop operating system.

4.2. Architecture

GoLightly comprises three primary application blocks:

- Model Processor 4.2.1
- Simulator 4.2.2
- Visualizer 4.2.3

FLOWCHART HERE?

4.2.1. Model Processor

The model processor (MP) is responsible for initialization of the simulator. When launching the simulator, a domain size and image file, containing a coded image of the desired dielectric, as well as a max ϵ are specified.

The MP allocates arrays to hold the dielectric properties for each Yee cell. These arrays are of the same dimensions as the domain, which may be different than the dimensions of the model.

Once the model image is loaded, the MP iterates through each element in the dielectric array. (See 4.2.1)

For each element:

1. Determine the normalized texel coordinate that corresponds to the current cell position
2. Read the red (R), green (G) and blue (B) color components from the image
3. If $R > 128$, this texel is part of a source. Add the cell to the list of sources.

```
for(int j = 0; j < media.Size.y; j++)
{
  int sourceY = j * height / media.Size.y;
  for(int i = 0; i < media.Size.x; i++)
  {
    int sourceX = i * width / media.Size.x;
    unsigned int sourceOffset = channels * (sourceY * width + sourceX);
    unsigned int mediaOffset = j * media.Size.x + i;
    unsigned char red =   bytes[sourceOffset + 0];
    unsigned char green = bytes[sourceOffset + 1];
    unsigned char blue =  bytes[sourceOffset + 2];
    // is this pixel part of a source?
    if (red > 128)
      sourceOffsets.push_back(mediaOffset);

    /// fill default waveguide material (parameter n)
    if (green > 0)
    {
      // interpolate n based on green value.
      media.HostArray[mediaOffset] = epsilonMax * green * 1.f / 255;
    }
  }
}
```

Generating a model from an image

4.2.2. Simulator

4.2.3. Visualizer

4.3. Modeling approach

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5.3. Meep vs GoLightly

5.4. Results

5.5. Limitations

Chapter 6

FUTURE WORK

future work...

REFERENCES

[1] Yee, K. Numerical solution of initial boundary value problems involving maxwell's equations in isotropic media. *IEEE Transactions on Antennas and Propagation 14*, 3 (1966), 302–307.