GPU Implementation of Hertzian Potential Formulation for Simulation of Nanosensors

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Abstract— **The time domain modeling and simulation of electromagnetic (EM) waves interaction with nanodevices, at high spatial andtime resolution, requires high computational power. In this paper we present an implementation of the Hertzian Potential Formulation (HPF) on the Graphics Processing Units (GPUs) through the NVIDIA's CUDA (Compute Unified Device Architecture)programming model. The results demonstrate that this GPU tool outperforms the CPU based HPF implementation, reaching a speedup from 30x to 70x.**

Keywords- ***GPU Implementation; Nanodevices; Hertzian Potential Formulation.***

I. INTRODUCTION

Recently a new method, the HPF (Hertzian Potential Formulation) [1]-[5], has been proposed for the simulation of full-wave propagation and reflection in the time domain. The main advantage of the HPF method is that it is computationally more efficient than the Yee FDTD [3]. In the one-dimensional domain it performs half of the computation, needing to solve only two instead of the four equations of the Yee's algorithm in the two-dimensional case [1]. Notwithstanding, accurate nanoscale simulations require great computing power that can be found not only in the expensive HPC (High Performance Computing) systems based on CPUs but also in the GPU (Graphics Processing Units) based solutions. In fact, a recent extraordinary evolution, from simple hardwired Video Graphic Array (VGA) controllers to highly multithreaded multiprocessors optimized for visual computing, made the GPUs mature massive parallel multiprocessors. In particular, they adopted wider bandwidth and a more general-purpose architecture that allows their usage as HPC systems with very low power consumption [8]. Moreover, given the wide integration in commercial off the shelf computers, they represent a powerful and cheap solution to computational science. GPU computing is being exploited in many scientific applications [6]-[8] with interesting results in the electromagnetic field and nanotechnology [9]-[10]. Much published work on EM computational simulations using the GPUs proves the growing interest in this powerful technology of the computational EM community [11]-[13].In this work we developed on GPUs a HPF based tool to accelerate the simulation of EM wave interaction with structures at nanoscale resolution. The time-domain HPF algorithm has been fully implemented on GPU [13], through a new computational pattern, to exploit their high computational power.

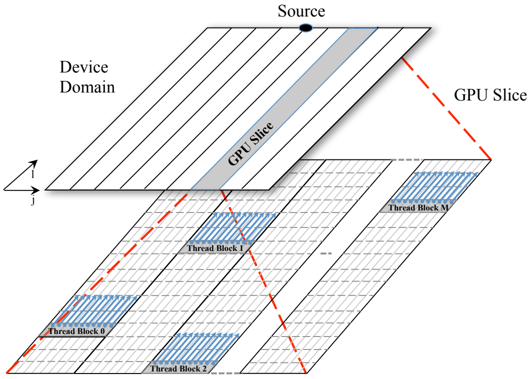

Fig. 1. Domain decomposition scheme: device domain is divided in slices provided to GPU's kernel. The data domain is further partitioned in blocks whose threads run HPF concurrently.

II. GPU/HPF RESULTS

In the new HPF all the possible electromagnetic field components, which can describe the scattering and radiation effect of a nanodefect, are defined by the Hertzian electric and magnetic vectors as:

$$\begin{aligned} \bar{\mathbf{E}} &= \nabla\nabla\cdot\bar{\Pi}_e - \varepsilon\mu\frac{\partial^2}{\partial t^2}\bar{\Pi}_e - \mu\frac{\partial}{\partial t}(\nabla\times\bar{\Pi}_h) \\ \bar{\mathbf{H}} &= \nabla\nabla\cdot\bar{\Pi}_h - \varepsilon\mu\frac{\partial^2}{\partial t^2}\bar{\Pi}_h + \varepsilon\frac{\partial}{\partial t}(\nabla\times\bar{\Pi}_e) \end{aligned} \qquad (1)$$

The eq. (1) is discretised and implemented by the GPU approach [14]: the points of the discretization belonging to a line parallel to the wave-front direction are updated consecutively, moreover, these lines are independent of each other and are updated in parallel by concurrent threads, one thread per line (Fig. 1). The HPF tool is used to simulate the behavior of a device with nanostructures organized in different positions (see Fig. 2). The HPF/GPU results show a good pattern of computing, moreover, the careful choice of shared memory usage can provide a speedup of 70x in single precision and almost 40x in double precision.

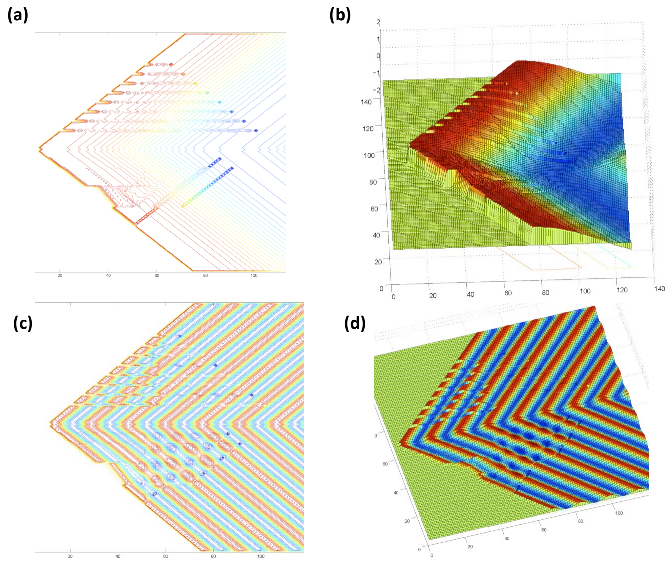

Fig. 2. HPF simulations: total electric field scattered by the nanodefects at different time steps: part of the electric field is back scattered and part is propagated along the waveguide. (a) Contour plot and (b) 3D plot obtained by exciting the nanodefects by a Gaussian pulse representing a plane wave propagation with dx=dy=10nm and $dt = dy \times \sqrt{(\varepsilon_{air} \times \mu_0)}$. (c) Contour plot and (d) 3D plot obtained by exciting the nanodefects by sinusoidal source working at λ = 1.55µm with dx=dy= 100nm and $dt = dy \times \sqrt{(\varepsilon_{air} \times \mu_0)}$

III. CONCLUSIONS

The goal of this paper is, starting from a defined code, to find a GPU matching approach. In particular the HPF code is performed in order to understand the limits of the GPU for similar EM codes. The CUDA platform and architecture has a low learning curve that allows every scientist to benefit of the extreme performance of the GPU computing. Nevertheless, smart tailoring of the code/algorithm to the resources available is required. n this work we demonstrate that with a few code modifications it is possible to perform simulations that otherwise require an expensive HPC cluster. The proposed tool is suited for the time domain simulation of nanodefects behaving as radiating nanosensors.

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