Modeling by Hertzian Potentials Regarding Wavefront Propagation in a Material with Nano-defects on a GPU based system

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In this work we present a new powerful tool based on the modeling of nano-defects in a generic material. This numerical tool considers the time domain Hertzian Potentials modeling implemented following the recent Compute Unified Device Architecture (CUDA) new parallel programming model, to be run on Graphic Processing Unit (GPU). The advantages of the scalar potentials and the efficiency of these massively parallel processors (NVidia's GPUs) provide a low computational cost and an high precision regarding the analysis of the scattering and coupling problems of a set of nano-defects arranged in a very long structure. In this case the aspect ratio limits related to long structure with nano-scale particles is overcame. The presented computational approach can simulate the combined effect of a set of nano-defects in a very long structure at a low hardware cost.

Born as accelerators for 2D and 3D graphic operations, the GPUs have evolved into a very attractive hardware platform for general purpose computing due to their extremely high floating-point processing performance, memory bandwidth and their comparatively low cost [4]. The rapid evolution of GPUs in performance, architecture and programmability can provide application potential beyond their primary purpose of graphic processing. High-End GPUs typically deliver performance of at least one order of magnitude higher compared to that of the CPU[5], while at the same time equipped up to 1 GB of GPU main memory. This commodity graphics hardware can become a cost effective, highly parallel platform to solve scientific problems and they have shown superior performance in some classes of applications and much faster evolution speed than Moore's law predictions for CPUs[4].
Since single precision might be insufficient for real applications, recently GPUs has improved their support for double precision floating-point (IEEE754 64 bit) with better performance. Especially when very low geometrical and physical variation occur as happens during the electromagnetic simulation of a nano-defect. Double precision may overcome this problem by supporting a good accuracy. Before the fabrication of a generic optical device is important to design and model accurately the structure in order to predict the EM behaviour: at optical frequencies the numerical solution is sensible to the variation of the geometrical parameters and a prediction of the geometrical imperfections of the fabrication process should be considered. An error of few nanometres generates different responses of the optical structure. For this reason sets of nano-defects can be considered in order to select a preferred EM response, but a very fine numerical discretization is requested. A good accuracy of the numerical solution is fundamental in order to simulate very small imperfection in very long structures. The numerical simulations of these imperfections distributed in complex 3D structures are characterized by a very high computational cost, and a normal personal computer cannot solve. Traditional numerical methods, such as Finite Difference Time Domain (FDTD), Finite Element Method (FEM), Beam Propagation Method (BPM), and others are limited about the accuracy of the EM solution. In particular we report below in details the critical configurations where the accuracy could fails at optical frequencies:

☐ Very thin dielectric layer in very long dielectric structure.
☐ Dielectric discontinuities.
☐ High bulk dimension in bulk-type structures.
☐ Nano-structures in long optical fiber.
☐ Singularity points.
☐ Nano-defects.

For a two-dimensional (2-D) problem the proposed Hertzian potential formulation (HPF) time-domain algorithm solves rigorously field by considering only two scalar coupled equations, by providing the requested accuracy. For the same problem, the conventional finite difference time domain (FDTD) algorithm solves for three field components which are correlated, by increasing of 50% the central processing unit (CPU) time[1][2].
In the New HPF Electromagnetic Model For Optical Waveguide, all the possible electromagnetic field components which can describe the scattering and radiation effect of a nano-defect are defined by the Hertzian electric and magnetic vectors as:

$$\overline{\mathbf{E}} = \nabla\nabla\cdot\overline{\Pi}_e - \varepsilon\mu\frac{\partial^2}{\partial t^2}\overline{\Pi}_e - \mu\frac{\partial}{\partial t}(\nabla\times\overline{\Pi}_h)$$

$$\overline{\mathbf{H}} = \nabla\nabla\cdot\overline{\Pi}_h - \varepsilon\mu\frac{\partial^2}{\partial t^2}\overline{\Pi}_h + \varepsilon\frac{\partial}{\partial t}(\nabla\times\overline{\Pi}_e)$$

by using the Hertzian potential scalars ψ^e , ψ^h the electromagnetic field will be performed by the following expression:

$$
\begin{aligned}
\overline{\mathbf{E}} &= \hat{x}A^e + \hat{y}B^e + \hat{z}C^e - \hat{x}\mu\varepsilon\partial^2{}_t\psi^e - \hat{y}\mu\varepsilon\partial^2{}_t\psi^e - \hat{z}\mu\varepsilon\partial^2{}_t\psi^e - \\
&\quad - \mu\partial_t(\hat{x}(\partial_y\psi^h - \partial_z\psi^h) + \hat{y}(\partial_z\psi^h - \partial_x\psi^h) + \hat{z}(\partial_x\psi^h - \partial_y\psi^h)) \\
\overline{\mathbf{H}} &= \hat{x}A^h + \hat{y}B^h + \hat{z}C^h - \hat{x}\mu\varepsilon\partial^2{}_t\psi^h - \hat{y}\mu\varepsilon\partial^2{}_t\psi^h - \hat{z}\mu\varepsilon\partial^2{}_t\psi^h + \\
&\quad + \varepsilon\partial_t(\hat{x}(\partial_y\psi^e - \partial_z\psi^e) + \hat{y}(\partial_z\psi^e - \partial_x\psi^e) + \hat{z}(\partial_x\psi^e - \partial_y\psi^e))
\end{aligned}
$$

The HPF model proposed is iterative, i.e. at each iteration time step the electromagnetic field information of each point of the planar waveguide must be properly updated. This update process requires data only from the previous two time steps, therefore all the points can be updated in parallel harnessing the GPUs massive parallelism. The workload for updating the fields data is shared between all the threads running on the GPUs following the phase shown below for each time step:

1. Update source
2. Update Mur boundary conditions
3. Update electromagnetic field

The phase 3) is computationally more intensive and is further subdivided into three parts:

4. Load previous time steps field values.
5. Computing of the new field values.
6. Store the result in memory

The key point in the CUDA implementation is to choose the best kernel block dimensions to get around the shared memory and bandwidth limitations obtaining significant performance improvement with the new GPUs implementation of at least one order of magnitude, as reported above. The Table 1 reports the comparison between features of the hardware used to perform the simulation by considering the optical power $|E|^2$ at a particular time step of a bidimensional ($n_x = 200$ $n_y = 200$) calculated matrix. In particular the simulation regards the propagation of an electromagnetic wave in a slab of dielectric material affected by a single nano-defect for a period of time Fig. 1.

TABLE I. FEATURES OF CPU AND GPU USED FOR SIMULATION

Hardware features	***Intel quad core Q9550***	***Nvidia GeForce GTX295***
Num cores	4	240
Clock rate	2.82 GHz	1.24 GHz
Main Memory	4 GB	1.749 GB

References

[1] Massaro A. and Rozzi T, “Rigorous time-domain analysis of dielectric optical waveguides using Hertzian potentials formulation,” *Opt. Express* 2006; 14(5): 2027-2036.

[2] Massaro A., Grande M., Cingolani R., Passaseo A., and De Vittorio M. “Design and modelling of tapered waveguide for photonic crystal slab coupling by using time-domain Hertzian potential formulation,” Opt. *Express.* 2007; 15(25): 16484-16499.

[3] NVIDIA CUDA Programming Guide 3.0, NVIDIA Corporation, 2010

[4] John D. Owens, David Luebke, Naga Govindaraju, Mark Harris, Jens Krüger Aaron, et al. “A survey of general-purpose computation on graphics hardware”, Computer Graphics Forum 34 (March) (2007) 80–113

[5] Olaf Schenk, Matthias Christen, Helmar Burkhart, “Algorithmic performance studies on graphics processing units” J. Parallel Distrib. Comput. 68 (2008) 1360–1369

Figures

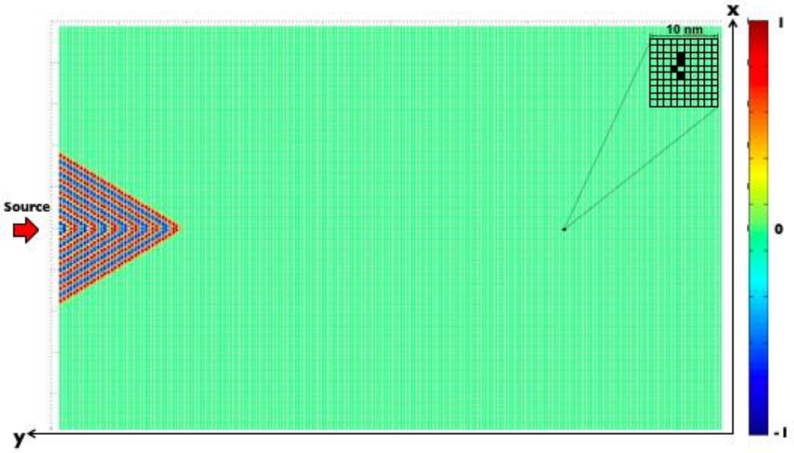

Figure 1. Planar waveguide: Wave front propagation after some timesteps. The simulation is performed by HPF approach implemented with CUDA on GPU.