Graphics-processing-unit-accelerated finite-difference time-domain simulation of the interaction between ultrashort laser pulses and metal nanoparticles

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Abstract. Metal nanoparticles (NPs) serve as important tools for many modern technologies. However, the proper microscopic models of the interaction between ultrashort laser pulses and metal NPs are currently not very well developed in many cases. One part of the problem is the description of the warm dense matter that is formed in NPs after intense irradiation. Another part of the problem is the description of the electromagnetic waves around NPs. Description of wave propagation requires the solution of Maxwell’s equations and the finite-difference time-domain (FDTD) method is the classic approach for solving them. There are many commercial and free implementations of FDTD, including the open source software that supports graphics processing unit (GPU) acceleration. In this report we present the results on the FDTD calculations for different cases of the interaction between ultrashort laser pulses and metal nanoparticles. Following our previous results, we analyze the efficiency of the GPU acceleration of the FDTD algorithm.

1. Introduction

Curiously enough, people know unique properties of nanoparticles for a long time. The Lycurgus Cup made in 4th century AD can be regarded as the first known example of gold nanoparticles optic properties [1]. Certainly, it took many centuries to understand physics of the observed phenomena. The classic problem of the scattering of an electromagnetic plane wave by a spherical particle was solved by Gustav Mie in 1908 [2]. Nowadays the development of the computers and computational methods enable us to solve previously unapproachable problems, but in the interaction of electromagnetic field with nanoparticles there are still many challenging questions. Especially since the development of laser processing technologies has reached the diffraction limit of far-field optics and the near-field effects have attracted the focus of research efforts.

Both theoreticians and experimentalists work on this topic. For example, an interesting study of plasmonic nanoablation of silicon in experiments with the use of femtosecond laser pulses incident on gold nanorods was presented in 2010 by Harrison et al [3]. In 2013 an attempt to construct a corresponding physical model was made by Robitaille et al [4]. Approaches for simulation of pump-probe experiments with metals are under active development [5].
2. Method

2.1. Model

In this work we use the open source finite-difference time-domain (FDTD) solver GSvit [6, 7]. It is focused on nanoscale optics, it supports graphics processing unit (GPU) acceleration by Nvidia CUDA technology and provides the graphical user interface for setup and visualization.

Computation volume spacing is set to 1 nm. The model consists of 100 nm gold or silver particle placed on the silicon substrate surface. The laser wavelength is 800 nm, the wave is incident normally to the surface. It is simulated by total-field scattered-field technique. Similar model has been described by Tanaka et al [8].

A metal nanoparticle is simulated by Drude-critical points model [9] and solved via the Recursive Convolution method. The silicon parameters are loaded from the Sopra n&k database.

Figure 1. Near-field enhancement calculated with the GSvit program: electric field near the gold nanoparticle (a) in vacuum; (b) on silicon substrate.
2.2. Hardware and performance issues
The calculations are performed on the computer with Intel Core i5-4210H CPU (dualcore Haswell architecture) and Nvidia GTX950M accelerator.

Of course, the computation time depends strongly on amount of output data, but we can compare values in very similar computations with the same output settings. Some advanced techniques (field sources and boundary conditions) significantly affect the performance of FDTD computation [10]. In our case, GPU computations with multithreading enabled take about 12.5 minutes of real time. The same simulation on the dual-core CPU takes about 4 times time more in comparison with the GPU variant. But not every problem fits into the GPU memory, which is limited by 2 Gb. In our case, we are able to run the computation of a 100 nm nanoparticle on GPU, but a 200 nm nanoparticles fits in the main DRAM memory only.

In this work we estimate the computational efficiency of the program using the general metric [11–13] “time-to-solution vs peak performance” (figure 2).

3. Discussion
The enhanced near-field distribution is presented on figure 1. One can see that the presence of a silicon substrate results in a strong change in the distribution of electric field. In the same time, the complete ablation simulation requires much more sophisticated models. The resulting FDTD-calculated data can be used as initial conditions for some other computational method, such as molecular dynamics [14]. This approach could result in the creation of new models for laser ablation.

Using the numerical FDTD model, one can go beyond analytic solutions of Maxwell equations. For example, one could get results for nonspherical or asymmetric nanoparticles of complex shape. It is possible to conduct computational experiments for a matrix of many particles on a silicon substrate, which have complex non-linear effects on each other. The figure 3 shows the computational domain configured for single nanorod and for the array of nanorods.
Figure 3. More complex geometries can be solved only using numerical computer calculations. The picture shows: (a) a cylinder that represents a common experimental case of a gold nanorod on a surface; (b) an array of nanoparticles.

4. Conclusion
In this paper, the illustration of the GPU-acceleration of FDTD calculations of the interaction between femtosecond laser pulses and metal nanoparticles is presented. We show the significant speed-up from the usage of GPU acceleration in the GSvit package. This computational method can solve problems with complicated and asymmetric initial conditions.

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References
[1] Terakawa M and Nedyalkov N 2016 Adv. Opt. Technol. 5 17–28
[2] Mie G 1908 Ann. Phys. 330 377–445
[3] Harrison R K and Ben-Yakar A 2010 Opt. Express 18 22556–71
[4] Robitaille A, Étienne Boulais and Meunier M 2013 Opt. Express 21 9703–10
[5] Povarnitsyn M E, Andreev N E, Apfelbaum E M, Itina T E, Khishchenko K V, Kostenko O F, Levashov P R and Veysman M E 2012 Appl. Surf. Sci. 258 9480–3
[6] Klapetek P and Valtr M 2010 Surf. Interface Anal. 42 1109–13
[7] Klapetek P, Valtr M, Poruba A, Neas D and Ohldal M 2010 Appl. Surf. Sci. 256 5640–43
[8] Tanaka Y, Nedyalkov N N and Obara M 2009 Appl. Phys. A 97 91–8
[9] Vial A and Laroche T 2008 Appl. Phys. B 93 139–43
[10] Vial I, Deinega A and Belouso S 2014 Comput. Phys. Commun. 185 1273–81
[11] Stegailov V V, Orekhov N D and Smirnov G S 2015 HPC hardware efficiency for quantum and classical molecular dynamics Parallel Computing Technologies, PaCT 2015 (Lecture Notes in Computer Science vol 9251) ed Malyskin V (Cham: Springer) pp 469–73
[12] Nikolskiy V P, Stegailov V V and Vecher V S 2016 Efficiency of the Tegra K1 and X1 systems-on-chip for classical molecular dynamics 2016 Int. Conf. on High Performance Computing & Simulation (HPCS) (Innsbruck, Austria: IEEE) pp 682–9
[13] Nikolskii V, Vecher V and Stegailov V 2016 Communications in Computer and Information Science 687 199–211
[14] Orekhov N D and Stegailov V V 2016 J. Phys.: Conf. Ser. 774 012104