МНРТИ 28.17.31

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SOLVING PHYSICAL MODELING TASKS USING A SUPERCOMPUTER

Abstract. The purpose of work is consideration of questions the use of modern high-performance systems and technologies for the solution of computing tasks in various sectors of economy and production. As the main objective distribution of electromagnetic waves in the inhomogeneous medium is taken. Such problems are successfully solved by numerical methods but more difficult analytical ones. For modeling boundary conditions of Bloch in the cylindrical system of coordinates have been set, the method of final differences and an algorithm Yee is chosen. We have simulated FTDT as the most suitable for high-performance calculations, in a package of MEEP established on the supercomputer of the L.N. Gumilyov Eurasian National University. The received results show high precision of calculations and also a possibility of search of new problems, a possibility of statement of other experiments with the choice of new environments for distribution of electromagnetic waves.

Keywords: computing devices, supercomputer, modeling, OpenMP, HPC.

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Аннотация. Целью работы является рассмотрение вопросов использования современных высокопроизводительных систем и технологий для решения вычислительных задач в различных секторах экономики и производства. В качестве основной задачи взято распространение электромагнитных волн в неоднородной среде. Такие задачи успешно решаются численными методами и сложнее аналитическими. Для моделирования были заданы граничные условия Блоха в цилиндрической системе координат, выбран метод конечных разностей и алгоритм Ия. Смоделирована FTDT, как наиболее подходящая для высокопроизводительных вычислений, в пакете MEEP, установленного на суперкомпьютере Евразийского национального университета им. Л.Н. Гумилева. Полученные результаты показывают высокую точность расчетов, а также возможность поиска новых проблем, возможность постановки других экспериментов с выбором новых сред для распространения электромагнитных волн.

Ключевые слова: компьютерные устройства, суперкомпьютеры, моделирование, OpenMP, HPC.

Түйіндеме. Мақаланың мақсаты қазіргі заманғы өнімділігі жоғары жүйелер мен технологияларды пайдалану мәселелерін қарау және экономика және өнеркәсіптердің әртүрлі секторларындағы есептеу міндеттерін шешу болып табылады. Басты мәселе ретінде біртекті емес ортада электромагниттік толқындардың таралуы алынған. Мұндай мәселелер сандық әдютермен табысты шешіледі, аналитикалық әдістер күрделірек. Блохтың шекаралық шарттары модельдеу үшін цилиндрлік координат жүйесінде берілді, соңғы айырмашылық әдісі және Ия алғоритмі таңдалды. Л.Н. Гумилев атындағы Еуразия ұлттық университетінің суперкомпьютерінде орнатылған MEEP пакетінде жоғары өнімді есептеу үшін ең қолайлы болып табылатын FTDT үлгісін жасадық. Алынған нәтижелер есептеулердің жоғары дәлдігін, сондай-ақ жаңа проблемаларды табу мүмкіндігін, электромагниттік толқындардың таралуына жаңа орталарды таңдау арқылы басқа эксперименттерді орнату мүмкіндіктерін көрсетеді.
Түйінді сөздер: компьютерлік құрылғылар, суперкомпьютерлер, модельдеу, OpenMP, HPC.

Introduction. HPC systems were originally designed and manufactured primarily for volumetric calculations that require resource-intensive workloads. But with the growth and accumulation of large sets of data, and in the future , the need for their storage, extraction, movement, analytics , machine learning and artificial intelligence, this also required the capabilities of HPC [1].

The development of supercomputers and computing centers is being carried out around the world, but to date , the largest number of supercomputer systems is in China, according to the statistics of their 202 centers. The largest center is the Chinese Sunway TaihuLight, it produces 93 quadrillion calculations per second. Another supercomputer from IBM is installed in China and is designed to accurately predict the quantitative characteristics of the air environment in the Beijing area. This computing system is among the ten fastest supercomputers in China [2]. In the USA of such centers are 144 and the largest one is Titan which consists of the mixed Opteron AMD processors (6274 processors) and NVIDIA K20x accelerators which located in Oak Ridge National Laboratory . Modern developments in the field of HPC are already directed to the creation of exascale computing systems, which productivity will be about one exaflops (exaFlops) [3]. On the basis of L.N. Gumilyov ENU is operated the Kazakhstan-India center for development ICT, which has an indian supercomputer PARAM, intended for both research and use in the educational process.

Methods of researches . In the last few years, there have emerged qualitatively new information and communication technologies, which continue to develop dynamically, introducing cardinal changes in all spheres of the economy, education and science. Embedded voice robots, artificial intelligence systems, advanced solutions for processing and data management, as well as cloud technologies. In the past, application developers relied on the clock frequency of microprocessors and optimization of a consecutive code for achievement of improvement of productivity . Today clock frequency microprocessors are reached due to heat removal and restriction of consumption of energy that becomes critical for use of overlapping in multinuclear processors. Also , development of scalable parallel algorithms and their realization is key aspect for receiving the improved representation on new generations of microprocessors.

One of the newest technologies is the blade technology from the company-developer of systems of supercomputers Hewlett-Packard (HP) [4]. It provides the required computing system in accordance with the workload at the optimum cost. By separating servers from the corresponding uplink channels, HP releases administrators from traditional infrastructure restrictions and simplifies management between servers and networks. This allows you to create pools of network, computing resources and storage resources that can be added, migrated or modified in minutes. Other scientific technology opened by researchers of the IBM company consists in creation of more effective way of the organization of channels of data exchange between kernels on a chip at the expense of light impulses through silicon layers, but not electric signals on wires. Use of light impulses allows to increase the speed of exchange of information by 100 times and to cut down electric power expenses by 10 times.

The fundamental problem of creating methods that make it possible to effectively use the aggregate power of many processors is the need to develop algorithms that have a substantial margin of internal parallelism at all stages of the calculation. Each step of solving a problem must contain a sufficient number of mutually independent operations, the execution of which is possible simultaneously on all processors allocated for calculation. Ideally all set of the operations necessary for the solution of a task should be distributed evenly between all processors throughout all time of performance of calculation. The specified problem, certainly, has the defining character, but it is not only one .

One of the most actively used methods of studying the processes occurring in complex multi-dimensional objects is the method of mathematical modeling. Often this method is the only possibility of studying complex nonlinear phenomena. Due to both time constraints and certain conditions, it is impossible to carry out some experiments, for example, a natural experiment in studying global climate changes, or studying the behavior of a substance under extreme nuclear explosion conditions. Expensive is also an experiment, which aims to determine the optimal modes of hydrocarbon production in oil fields. Thus, where a natural experiment is impossible, a computational experiment is necessary. Within its framework, a mathematical model of the phenomenon is created. The use of methods of mathematical physics leads to the description of the object of investigation by a system of nonlinear multidimensional partial differential equations, the solution of which is determined by numerical methods. The continuous medium is replaced by a discrete analogue – the finite grid in time and space. Differential equations acting in a continuous space are replaced by algebraic ones acting in the discrete space of a difference grid or finite elements.

The solution of algebraic equations is entrusted to high-speed computing systems. The accumulated experience of using multiprocessor systems for modeling physical and technological processes is focused on parallel systems of average performance, containing a relatively small number of processors. Upon transition to computing systems, the number of processors in which is estimated in hundreds and more, creation of other means of processing of large volumes of data is required. Parallel computing is a multithreaded calculation directed to solving a uniform task. Each stream of calculations is performed independently of others, allowing a mutual exchange of data or even the presence of a common address space. And, as already noted, the main thing in this process is the correct selection of parallelization methods, analysis of the algorithm of the problem, that whether the given task is divided into parts of equal complexity that can be executed independently of each other [5-7].

Modern ordinary computers allow to carry out parallel calculations as, at least, contain four cores and can be used for any tasks in which separate parts can be distinguished:

- processing of large volumes of experimental data. If you need to perform the same operations with these data, you must divide them into streams, which leads to faster work.

- obtaining characteristics of complex objects. To do this, you need to run the same model many times, and, therefore, you can parallelize these processes.

- acceleration of huge system models. Also, the model can be divided into parts, run each part many times and on different cores.

In the process of parallelizing a task, participate such programs as the scheduler, the task manager, the time allocation functions of the processors between several tasks, and the functions for sharing the resource space, and others. The scheduler divides the bulk task into parts and runs them on different cores, and not necessarily the tasks should be the same , the main thing is that each of these tasks is solved on its computing core. The task manager automatically processes a number of components and determines for each of them the start time, as well as the delivery of input files to the execution node, monitoring the execution and delivery of the result. It happens that if you have experimental data, it is difficult to create a model, because the model does not work as an experiment, and you need to select parameters to it. This means that the program runs the model first with one set of parameters, then it looks whether the desired result is obtained, if not, it changes this set of parameters, again simulates, and so on. At the same time, interaction with the rest of the program occurs through standard messaging facilities such as MPI and PVM.

Another of the most famous models of parallel programming is Open MP, which for 20 years has passed a great evolutionary path from the first computer system, consisting of 1952 cores, with a clock frequency of 200 MHz and a performance of 1.34 Tflopfs to a system consisting of 10 million cores, a frequency of 1.45 GHz and a capacity of 125,436 Tflopfs. Also during this period there was a merger of Fortran and C/C ++ specifications, implementation of SIMD parallelism instructions, support of cycle tasks, priority tasks, parallelization of irregular applications built on non-regular applications and data structures such as graphs [8].

Main results. Modeling of electromagnetic waves propagation in the non-uniform materials was solved on the Param-Bilim supercomputer, located in the Kazakhstan-India High Performance Computing Center. This supercomputer is developed by the Indian company C-DAC and equipped with processors 5110p Xeon Phi, NVIDIA Kepler K20x. It is known that Maxwell’s equations are the cornerstone of all electromagnetic phenomena, and their decisions are applied to a wide range of tasks including for problems of distribution of electromagnetic waves in the non-uniform environment. The most widespread method is the method of final differences on the displaced grids – Finite Difference Time Domain (FDTD) known as an algorithm Yee [9-11]. To date, there are many publications on using of various aspects of the FDTD method and their full-scale development grows with the growth of computer performance. The main advantage of this method is the possibility of calculating electrodynamic objects with inhomogeneous , anisotropic and nonlinear media with arbitrary shape of the boundaries [12]. The MEEP (MIT Electromagnetic Equation Propagation) software package is a free product for finite-difference modeling in the time domain of electromagnetic systems [13].

MEEP allows to simulate one-dimensional, two-dimensional and three-dimensional systems in cylindrical coordinates. For modeling, three boundary conditions have been established: the periodic boundaries of the Bloch condition, the metal walls and the absorbing boundary conditions in the form of PML layers. In problems with ordinary periodic boundary conditions in a cell of size L, the field components satisfy f(x + L) = f(x). And the Bloch boundary conditions are a generalization, where f(x+L) = eikLf(x) for some wave vector k of the Bloch. A simpler boundary condition in MEEP is a metal wall where the fields at the boundaries are zero. In fact, it is possible to place perfect metallic materials anywhere in the computational cell, for example, to simulate metallic cavities of arbitrary shape. To simulate open borders, perfectly matched layers (Perfectly Matched Layers - PML) are used to absorb all the waves that fall on them, without any reflections. The main parameters of the experiment are given in Table 1.

To perform simulation a classical approach based on the differential space-time formulation of the Maxwell equations is applied to the FDTD method. The grids for electric and magnetic fields are shifted in relation to each other in time and space by half the sampling step for each of the variables. Finite-difference equations allow the calculation of the electric and magnetic fields at the current time, and for the given initial conditions, the computational procedure unfolds the solution in time from the origin with a given step.

Table 1

No	Options	Value
1	The size of the calculation area	20x20
2	Boundary conditions	PML
3	Environment of the region	Vacuum
4	Model of material object, dimensions	Cone with a radius 2 and 0,5

5	Location of the object relative to the calculation area	x = - 4;
		y = 0;
		z = 0;
		h = 12;
		axes = (1;0;0)

6	Material type of the object, transmittivity	epsilion = - infinity
7	Source type, frequency	Continuous – srs, length of wave = 3, width = 5
8	Source location	x = 8.8; y = 8 8
9	Calculation time	25.6 s
10	Grid resolution	10

Conclusion. The aim of the simulation is to search for patterns of propagation of electromagnetic waves in a medium with inhomogeneous properties, the study of these regularities is an actual problem, on the principles of electromagnetic radiation, modern mobile communication devices, Wi-Fi, radars, telescopes in space observatories, etc. have been created. Thanks to a large number of applications for electrodynamics problems, it is possible to set and solve new problems for Maxwell's equations with the choice of new media and sources of wave propagation [14].
We thank the Kazakhstan-Indian center Param-Bilim for the provided resources for the solution of problems of modeling of electromagnetic waves in the non-uniform environment.

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