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REVIEW ARTICLE

PARALLEL PROGRAMMING MODELS FOR CALCULATING THE PHYSICAL CHARACTERISTICS OF COMPOSITES

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ABSTRACT

This article reviews the performance of supercomputers. The increase in computational performance is also provided through parallel programming, the development of which is represented by a set of high-level programming languages, the emergence of new architectures and distributed and cluster systems. The article presents a numerical simulation of the calculation of the physical characteristics of the composites using the OpenMX package. At the same time, the use of parallel programming methods led to a significant increase in computing performance.

KEYWORDS

Programming models, parallel computing, performance, algorithm

1. INTRODUCTION

Today in the field of a hardware development is reached the organization of independence of operation of the computers of different devices (the processor and devices of input-output), there was a multilevel memory, were improved architecture of processors (a superscalarity, pipelining, dynamic planning) [1]. Though it is considered that many possible ways of improvement of processors are almost exhausted (as the possibility of further increase in clock frequency of processors is limited to a number of complex technical problems), nevertheless, the processors have gone a long way in evolution.

Among the various classifications of computing systems, the Flynn classification is key, but the most perspective direction in increasing productivity is the organization of multiprocessing computing devices.The latest developments of supercomputers have improved processors, a large number of cores and an optimized architecture. Currently, most supercomputers have a cluster architecture consisting of more than 1000 nodes. All nodes are connected by a high-performance network that can transmit up to 40 Gbit/s, which ensures high performance on computing tasks like LINKPACK [2].

A new generation of supercomputers, focused on working with big data and artificial intelligence, is created according to principles that are significantly different from those that were laid in high-performance cluster systems until 2017. High-performance computing plays an important role in the field of scientific computing, allowing you to perform the solution of scientific problems faster and more qualitatively. On the basis of L.N. Gumilyov ENU has an Indian-made supercomputer (figure 1) with the following main characteristics:

- HP DL380p G8;
- 2 X Intel Xeon E5-2670 Processor (2.6 GHz, 8 Core);
- Nvidia GTX780.

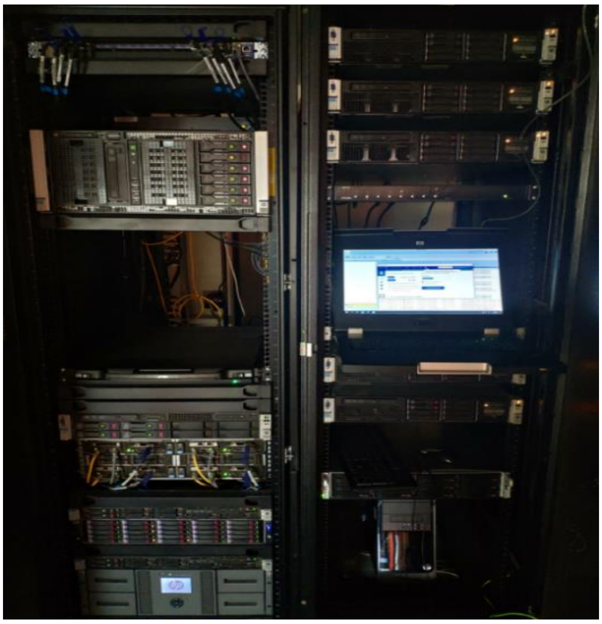

Figure 1: The supercomputer at L.N. Gumilyov ENU

The hardware of the supercomputer is equipped with the LINUX operating system, with support for parallel computing and HPC. This OS has an application for Computational Physics and Materials Modeling, such as OpenMX (Open source package for Material eXplorer) is a program package for nano-scale material simulations based on density functional theories (DFT), norm-conserving pseudopotentials and pseudo-atomic localized basis functions. Since the code is designed for the realization of large-scale ab initio calculations on parallel computers, it is anticipated that OpenMX can be a useful and powerful tool for nano-scale material sciences in a wide variety of systems such as biomaterials, carbon nanotubes, magnetic materials, and nanoscale conductors [3].

2. PERFORMANCE AND PARALLEL PROGRAMMING MODELS

To achieve increase in productivity depending on type of tasks and their complexity, it is possible the next ways:

- algorithms optimization;
- parallelization (instructions, threads, machines);
- specialized hardware decision.

Optimization algorithms are suitable for problems that can be solved by classical parallel algorithms [4-6]. An example of optimization of the algorithm is one of the approaches to the improvement of the texture compression algorithm based on cluster analysis, which is used in the NVIDIA DXT compressor, as an example given in article [7]. Examples of parallelization and their variants of parallelism are presented in [8]. The most common method is using parallelism using multiple cores or compute nodes.

In a study, an example of using a specialized hardware solution is presented [9]. Clusters, organization issues, resource sharing, software models for high-performance computing, comparative launching characteristics of various applications on CPU and GPU, on two computing clusters are considered. The specialized equipment includes XeonPhi, FPGA and, accordingly, other programming languages HDL, VHDL, Verilog [10]. The most important characteristic of parallel computing is program execution time. The laws of Amdahl and Gustafson-Barsis, prove some theorems relating the temporal characteristics [11].

Conditionally parallel programming can be divided into four groups:

- process/channel;
- message passing;
- data parallel;
- shared memory.

Parallel data processing becomes the main solution for increasing productivity. Dependence of programming models and architectural solutions for parallel data processing is interdependent. This connection is most clearly seen in the following programming models: a model with data parallelism, a model with shared memory, and a model based on message transmissions. One of the mechanisms for executing parallel processes was multi-thread programming. OpenMP represents the concept of threads and is often implemented by them. An OpenMP program is serial-parallel. Consecutive plots are performed by the root process. For the execution of parallel sections are formed threads.

3. PHYSICAL CHARACTERISTICS OF COMPOSITE MATERIALS

Composite materials and their diversity have a wide practical application. The need to develop and study the physicomechanical properties of composite materials leads to an increase in research activity over the past few years [12]. Composition called multicomponent materials consisting of a plastic base (matrix) and filler (reinforcing component). The matrix ensures the preservation of the required shape and size, binds the filler, has continuity in volume and determines the technological parameters of the material obtained. The filler takes the external load, is a component divided in the volume of the material and imparts special properties. Between the phases (components) of the composite there is a pronounced interface.

One of the main properties of the composite is high strength and lightness of the material. These qualities are determined by the choice of the optimal parameters of the process, the technical level of the equipment used, the availability of reliable methods for monitoring and predicting their behavior. Methods for calculating the strength of composites are effectively used in computer programs for predicting the physicomechanical characteristics of structures. For example, software using a graphics processor, speeds up the process of subtraction, allows you to change the parameters and see the results of changes in the properties of materials, reduces the time to test the obtained materials during research, and establish a more accurate percentage of the filler, which ultimately affects the reduction of production costs. The main types of composites are presented in table 1.

Table 1: Types of composites

Matrix phase/reinforcement phase	Metal	Ceramic	Polymer
Metal	Powder metallurgy parts – combining immiscible metals	Cermets (ceramic-metal composite)	Brake pads
Ceramic	Cermets, TiC, TiCN Cemented carbides – used in tools. Fiber-reinforced metals	SiC reinforced Al2O3 Tool materials	Fiberglass
Polymer			Kevlar fibers in an epoxy matrix
Elemental (carbon, boron, etc.)			Rubber with carbon (tires) Boron, Carbon reinforced plastics
	MMC's Metal Matrix Composites	**CMC's** Ceramic Matrix Composites	**PMC's** Polymer Matrix Composites

The experiment was carried out with the establishment of these characteristics for the use of polymer composites. Layered composite materials are widely used in modern production due to the high values of specific strength and stiffness. The non-linear mechanical characteristics of the composite material make the design process more time consuming compared to traditional products.

4. MATHEMATICAL MODEL

In general, the task of modeling the strength of composites is to obtain the strength fields and select the appropriate coefficients.

Construction of the strength function of the composite $\sigma = f(v)$ from the volume content of the filler v (figure 2). The strength of the composite is considered from the point of view of high resistance to thermal loads [13].

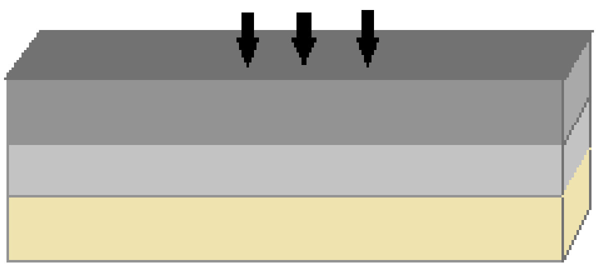

Figure 2: Load distribution in a three-layer composite

1. The strength of the composite σ_c at a certain content of the filler v can

be characterized by the expression:

$$\sigma_c = \sigma_p - \sigma_d \quad (1)$$

where σ_p is the strength of the defect-free composite with regard to hardening, σ_d is the softening of the composite due to its defectiveness.

2. There is such an optimal filler content v_0, at which the strength of the composite material is maximum. It is from equality

$\frac{d\sigma_p(v_0)}{dv} = \frac{d\sigma_d(v_0)}{dv}$, which is equivalent to $\frac{d\sigma(v_0)}{dv} = 0$.

For any deviation of v from v_0, we have $\frac{d^2\sigma_p}{dv^2} < 0$; $\frac{d^2\sigma_d}{dv^2} < 0$, which corresponds to the condition of maximum of the function σ_c with optimal filling. Summing the expansion in a Taylor series σ_p and σ_d expression (1) takes the form:

$$\sigma_c = \sigma(v_0) - 0{,}5a|\Delta v|^2 \quad (2)$$

where $\sigma_c(v_0) = \sigma_p(v_0) - \sigma_d(v_0)$ is a maximum strength of the composite material, $a = \frac{d^2\sigma_p}{dv^2} + \frac{d^2\sigma_d}{dv^2}$.

According to $\frac{d\sigma_p(v_0)}{dv} = \frac{d\sigma_d(v_0)}{dv}$, the linear term in the dependence (2) is absent, therefore, for any deviation $\Delta v = v_0 - v$ from the optimal value v_0, the strength of the composite decreases.

3. The strength of the composite material σ_c depends on the strength of the matrix in the array σ_m (H/m^2) and the surface film matrix σ_s (H/m^2)

$$\sigma_c V_c = \sigma_m V_p + \sigma_a S_{cl} \quad (3)$$

where V_c and V_p are the volumes of the composite and the bulk phase of the matrix, respectively. S_{cl} is the total surface area of cluster regions with a film matrix. Expression (3) is an analogue of the Ioffe equation, reflecting the dependence of the breaking load of the sample on the cross-sectional area and perimeter.

5. Take the volume of the composite for a single $V_c = 1$. Further, applying the formulas for expressing the volume content of the filler (spherical particles), expression (3) takes the form:

$$\sigma_c = \sigma_m(1 - 1{,}48v) + \sigma_a s_{cl} \quad (4)$$

where $s_{cl} = S_{cl}/V_c$ is the specific surface area of cluster formations.

6. Since the number of supercritical clusters K does not change, it is permissible to accept the n-cluster hypothesis. We simplify the model, assuming that all clusters have the same number of particles. Expressing the volume, surface area of cluster formations through the characteristics of their constituent particles, expression (4) takes the form:

$$\sigma_c = \sigma_m - 1{,}48\sigma_m v + 4{,}8K^{1/3}\sigma_s v^{2/3} \quad (5)$$

7. As a result of analysis (5), according to the test results of polyester, epoxy, furan composites for strength under uniaxial compression, it was found that the surface strength σ_s significantly depends on the dispersion of the filler and increases linearly with this parameter:

$$\sigma_s = \sigma_{s0} + a_s s_u \quad (6)$$

where σ_{s0}, a_s are constant values, s_u is the specific surface of the filler. For the studied composites, the numerical values of the constants σ_{s0}, a_s were found:

$\sigma_s = 21 + 0{,}02s_u$ for epoxy composites, $\sigma_s = 17 + 0{,}02s_u$ for polyester, $\sigma_s = 13 + 0{,}02s_u$ – for furan. The coefficient did not change its value and for all studied composites remained a constant $a_s = 0{,}02\ MH/m^3$. This shows that the increase in surface strength is mainly due to the geometric parameter characterizing the magnitude of the total surface of the reinforcing filler.

8. Taking into account the established dependence (5), equation (6) is transformed into a more applicable form:

$$\sigma_c(v) = \sigma_m - 1{,}48\sigma_m v + 4{,}8K^{1/3}(\sigma_{s0} + a_s s_u)v^{2/3} \quad (7)$$

Strength analysis of layered composites is carried out taking into account the orientation and thickness of each layer according to all modern criteria for destruction. In this case, it is possible to work with both surface and solid layered geometry (in the case of thicker structures). Таким образом, результаты измерения напряжений зависят от физических постоянных материала.

To write the algorithm, two parallel programming technologies, OpenMP and MPI + OpenMP, were used, thanks to which we obtain the following time optimization (fig. 3): with a sequential program, the time spent on the calculation was 341.2981 seconds, when using two threads already reduced to 166.8486 seconds. As for the time for the iteration, it decreased from 215.2463 seconds to 38.43916 seconds. These algorithms were calculated on the L.N. Gumilyov ENU supercomputer.

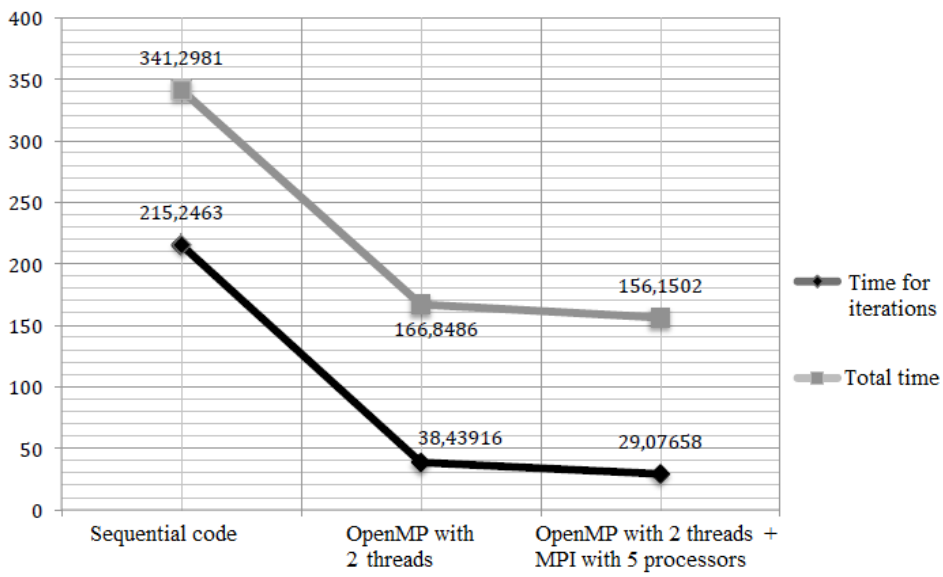

Figure 3: Time optimization on different codes

The main advantage of this model is the lack of synchronization with common variables, that allows to simply increase the computing power.

5. CONCLUSION

Questions of ensuring productivity of processors has been widely recognized. Lots of existing works focused on parallel applications, architectures software and hardware, development of heterogeneous systems and other. Also, many works are devoted to problems which can cause deterioration in productivity, for example, job failure, power consumption etc. Parallel programming models are key to increase the productivity of parallel software. The degree of complexity of the problem being solved and the amount of data computed determines the choice of high-performance systems and their application.

The strength calculations of polymer composites were performed on the OpenMX package with support for MPI and OpenMP (--with-mpi --with-openmp), which allowed us to speed up the calculations and at the same time use more memory for calculations. Experiments in which the same problem is solved by an increasing number of processors do not quite accurately show the effectiveness of the system. In practice, additional computational resources can be used not only to solve existing problems in less time, but also to solve more complex problems in the same time.

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