

ANNOTATION

dissertation work of Sakypbekova Meruert on the topic: “Optimal memory layouts and communication patterns for parallel unstructured CFD codes”, submitted for the degree of Philosophy Doctor (PhD) in the specialty “6D075100 – Computer Science, Computer Engineering and Management ”

Relevance of the research topic. High-precision hydrodynamic modeling is usually associated with large computational requirements, sharper with each new generation of supercomputers. However, significant research is currently needed to uncover the processing power of advanced systems, referred to as pre-ecaflops systems, based on more advanced architectures. On a computer, parallelization of proprietary code for numerical computations is becoming commonplace. With the development of numerical solvers and the complexity of problems, the possibilities of parallel computing also grow. Various proposed schemes are used for parallelization using CPUs and GPUs. Previously, high-performance computing was performed in large clusters of computers, each of which could execute a small number of parallel threads. However, in the last decade, general purpose graphics processing units (GPUs) have shown great performance gains. Each GPU can execute thousands of threads at the same time with lower overhead. While this type of performance was originally designed to support video applications, it has become essential for scientific computing and speeding up machine learning algorithms.

CFD's current merit is the development of new and improved devices and system structures, as well as the optimization of existing equipment through computer simulations, resulting in increased efficiency and reduced operating costs. With the rapid development of computer technology, computational fluid dynamics (CFD) plays an important role in the analysis of aerodynamic characteristics, efficient design and investigation of complex flow mechanism. High-performance computing on general purpose graphics processing units (GPUs) with complex coupled simulations with non-trivial domain decompositions using Hilbert space filling curve (SFC) using unstructured computational grids.

The purpose of the dissertation work: The purpose of this work is to apply the Hilbert space filling curve scheme using an unstructured computational grid for various resource-intensive physical and technical problems on general-purpose graphic processors. The proposed scheme makes it possible to increase the efficiency of complex simulation based on performance measurements during simulation. The approach makes it possible to automate the distribution of the computational grid into one-dimensional arrays that can be used to efficiently distribute the workload.

The objectives of the research, realizing the purpose of the dissertation work:

- numerical study of the effectiveness of high-performance computing on general-purpose graphics processing units for circulation incompressible viscous flow in a cavity;

- numerical study of the efficiency of high-performance computing on general-purpose graphics processing units for problems of incompressible viscous flow behind a backward step using structured computational grids;
- numerical study of the efficiency of high-performance computing on general-purpose graphics processing units for problems of incompressible viscous flow behind a reverse step using Hilbert space filling curve using unstructured computational grids.

The object of research is high-performance computing on general-purpose GPUs with a Hilbert space filling curve scheme for unstructured computational grids for various resource-intensive physical problems.

Research methods. In this dissertation work, methods are proposed that are a new tool in the study of load distribution on a different processor when using unstructured computational grids. The scheme of the Hilbert space filling curve makes it possible to increase the efficiency in decomposing the computational grid into domains.

For numerical calculations, the work uses parallel numerical algorithms on general-purpose graphics processors, and the results obtained are compared with the calculated and experimental data of other well-known authors.

The subject of the study is efficient high-performance computing on general-purpose graphics processing units using CUDA technology for numerical solutions of the Poisson equation, circulating incompressible viscous flow in a cavity, and problems of incompressible viscous flow behind a backward step.

Theoretical and practical value. The results presented in this paper can be widely applied in solving important applied problems that are associated with numerical simulation on general-purpose graphics processing units using CUDA technology. The developed schemes and numerical algorithms designed for numerical simulation on general-purpose graphics processing units make a direct contribution to the development of science and information technology in the country.

The practical value of this dissertation is that the Hilbert space filling curve (SFC) scheme used for unstructured computational grids on general-purpose graphics processing units allows not only to obtain a significantly “fast” result compared to sequential calculations, but also expands the possibilities of implementing labor-intensive methods and algorithms for solving important applied and fundamental problems.

Scientific novelty. We have developed an optimal memory layout and parallelization communication patterns for unstructured computational grids on general-purpose graphics processing units to increase the performance efficiency of massively parallel computing. So this approach is applied to various resource-intensive physical problems when using an unstructured computational grid by the Hilbert space filling curve (SFC).

Provisions for defense:

- results of a numerical study of the efficiency of high-performance computing on general-purpose graphics processing units for various resource-intensive physical problems;

- substantiation of the use of various memory layouts and communication patterns on general-purpose graphics processing units for various resource-intensive physical tasks;
- efficient use of high-performance computing scheme on general-purpose graphics processing units with complex coupled simulations with non-trivial domain decompositions using Hilbert space filling curve (SFC) using unstructured computational grids.

Scope and structure of work. The total volume of work is 90 pages. The dissertation work consists of an introduction, 5 sections, a conclusion, a list of sources used from 84 titles, 2 appendices, includes 46 figures and 7 tables.

The main content of the work. This work is presented in the following order.

The introduction discusses the relevance of the chosen topic of the dissertation work, the purpose, object, subject and objectives of the study. The results of the research, their scientific novelty and practical significance are described.

The first section was dedicated to the analysis of modern high-performance computing systems for applied problems. The calculations with the help of multi-core CPUs and the basic principles of calculations on the GPU are described. At the end of this chapter, we present an analysis and evaluation of the efficiency of high-performance computing on the CPU and GPU.

The second section presents a mathematical model for modeling. This chapter summarizes the basic equations of hydrodynamics: the equation of continuity, the equation of motion of a continuous medium. The nondimensionalization and discretization of the Navier-Stokes equation are described.

In the third section, the solution of the Poisson equation in a certain rectangular domain was considered, covering a wide class of applied problems. Using this equation, a numerical calculation was presented on the CPU and GPU, based on this calculation, a comparative analysis was made, which showed the effectiveness of the parallel numerical algorithm.

In the fourth section, the problem of an incompressible viscous flow in a cavity is considered. Based on this task, the result of efficiency on the GPU was obtained using different block sizes. Comparative analysis of CPU and GPU performance was made, showing a significant increase in GPU speed. This computational time comparison shows the advantage of GPU technology in solving computationally intensive engineering problems. An analysis of the number of threads per block, perhaps the most important parallelization parameter in CUDA, shows that there is an optimal value. This result is a simple but powerful CUDA optimization technique that greatly affects the overall processing time.

The fifth section presents the results of mixed-convective heat transfer in the process of laminar two-dimensional flow in a vertical channel in structured and unstructured meshes. A wide range of inlet flow conditions and wall temperatures is studied numerically, covering the region from a purely forced convective flow. This section shows the result of using problems of incompressible viscous flow behind a reverse step on structured and unstructured meshes, based on the application of parallelization in CUDA technology using the Hilbert Space Filling Curve (SFC)

scheme. The results of this study showed agreement on structured and unstructured meshes, which was applied to an unstructured mesh for the first time.

In conclusion, the conclusions of this dissertation work are presented.

Publication list:

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2. Issakhov, A., Abylkassyomova, A., Sakypbekova, M. (2019). Applications of Parallel Computing Technologies for Modeling the Flow Separation Process behind the Backward Facing Step Channel with the Buoyancy Forces. *Communications in Computer and Information Science*, CITech 2018, CCIS 998, 2019, pp. 97–113,

3. Исахов А.А., Сақыпбекова М.Ж. Құрылымды емес торды қолдануда есептеу гидродинамикасындағы параллельді технологиялардың теориялық негізі. Конференция «XLI Международная научно - практическая конференция на тему; «Инновационные технологии на транспорте: образование, наука, практика»», уровень Международный, КАЗАХСТАН, КазАТК имени Тынышпаева, г. Алматы, 03.04.2017-04.04.2017

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