ANNOTATION

of dissertation work of Abylkassymova Aizhan on the topic: "Potential of hybrid OPENMP/MPI parallelization strategies for HPC software", submitted for the degree of Doctor of Philosophy (PhD) in the specialty "6D060200-Computer Science".

Computer science technologies are gaining popularity every day, as today the era of high-performance parallel computing systems has begun. For this reason, the issue of accelerating and processing and analyzing large amounts of data is acute. There are several ways to solve this problem, such as multi-core machines, supercomputers, or grid systems. Parallel algorithms are also used for processing, modeling and visualization of both original and transformed data. Depending on the technologies used in the construction of parallel programs, the architecture of computing systems is built. For example, support for multithreading and development of programs for specialized systems (NVIDIA CUDA, OpenCL, OpenACC, OpenMP).

As is known, the use of parallel technologies can be due to such reasons as modeling real physical problems described by systems of differential equations in partial derivatives. For instance, the flow of a viscous incompressible medium is one of the important problems of mechanics. In fact, it is very difficult to achieve high efficiency for large-scale parallelized tasks. Since even the slightest imbalance can lead to undesirable results in overall performance. Dynamic load balancing (DLB), in turn, improves the efficiency of complex modeling with non-trivial domain decomposition. This possibility is provided by the Hilbert Space Filling Curve (SFC) at a coarse level. Since it is necessary to take into account various numerical methods, as well as various computational costs this schema automatically assigns weights to estimate the overall workload distribution. Due to the inability of this evaluation procedure to capture local workload changes, the overall SFC-based load balancing approach may not be optimal. Therefore, the DLB incremental diffusion algorithm is based on SFC separation, which allows to customize the domain decomposition. Simulations for various physical processes in complex domains demonstrate the effectiveness of DLB schemes for various large-scale related problems. A detailed performance analysis showed the need to use the DLB method to directly determine load imbalances, which, for example, are caused by individual computational efficiency depending on the composition of the local workload, scalability of individual program codes. In addition, the strong scaling experiment showed performance improvement with increasing degree of parallelism when a priori estimated computational weights are used for the initial split.

Objectives of the study. The aim of this work is to apply the dynamic load balancing (DLB) scheme, which makes it possible to increase the efficiency of complex modeling for various physical and technical problems. A minimal intrusive method has been proposed for estimating computational weights based on performance measurements during simulation. The approach allows to

automatically determine the appropriate weight parameters that can be used to estimate the overall distribution of the workload.

Study object. The object of research is high-performance computing using the method of dynamic load balancing for various physical problems.

Research methods. The methods proposed in the dissertation work are a new tool in the study of the problems of load distribution on various processors. Dynamic Load Balancing (DLB) scheme that improves the performance of complex modeling with non-trivial domain decompositions.

For numerical calculations, parallel numerical algorithms have been used in the work, and the obtained results are compared with the calculated and experimental data of other well-known authors.

Theoretical and practical value. The results of this work can be widely used in solving important applied problems related to numerical simulation on high-performance cluster machines.

The developed schemes and numerical algorithms make a direct contribution to the development of science in distributed computing and in the field of computer science in the country. The practical value of the work lies in the fact that the developed scheme of dynamic load balancing (DLB) on high-performance systems of great practical importance allows not only to obtain a significantly “fast” result compared to sequential calculations, but also expands the possibilities for implementing labor-intensive methods and algorithms for solving important applied and fundamental problems.

Scientific novelty. A dynamic load balancing (DLB) scheme has been developed to improve the performance efficiency of massively parallel computing. So this method with different numerical methods and different computational costs per subdivided cell has been obtained using the Hilbert Space Filling Curve (SFC) at a coarse level.

Using the constructed parallel numerical algorithm, the following were performed:

- numerical study of the efficiency of high-performance calculations for problems of flow behind a backward step;
- numerical study of the efficiency of high-performance computing using hybrid parallel algorithms for air flow problems in a complex nasal area;
- hybrid parallel numerical computation using various domain decomposition methods;
- hybrid parallel numerical computing using the method of dynamic load balancing;
- evaluation of the efficiency of hybrid parallel numerical computing using various methods of domain decomposition;
- evaluation of the effectiveness of a hybrid parallel numerical algorithm using the method of dynamic load balancing;
- comparison of the received results of modeling with numerical data and experimental data of other authors is carried out;

- the analysis of the obtained results of hybrid parallel numerical computing and hybrid parallel numerical computing using the method of dynamic load balancing was carried out;

Defense provisions. The work contains the following results:

- results of a numerical study of the efficiency of high-performance computing for flow problems behind a backward-facing step.
- results of a numerical study of the efficiency of high-performance computing when using hybrid parallel algorithms for problems of air flow in a complex nasal region.
- results of hybrid parallel numerical computation using different domain decomposition method.
- results of hybrid parallel numerical computation using dynamic load balancing method.
- results of evaluating the efficiency of hybrid parallel numerical computation using various domain decomposition methods.
- results of evaluating the efficiency of the hybrid parallel numerical algorithm using the dynamic load balancing method.
- comparison of the obtained simulation results with numerical data and experimental data of other authors is carried out.
- analysis of the obtained results of hybrid parallel numerical computation using the method of dynamic load balancing.

The structure and scope of the dissertation. The dissertation consists of designations and abbreviations, introduction, five chapters, conclusion and list of references. It is presented on 122 pages, the list of used sources contains 126 titles.

The main content of the work. This work is organized as follows:

The first chapter provides descriptions of various technologies for high performance computing.

The second chapter has a detailed description of the analytical models of the main characteristics of the parallel algorithm.

The third chapter provides a detailed description of the mathematical formulation of the basic equations for modeling the problem.

In the fourth chapter, numerical studies of the efficiency of high-performance computing for backward-facing flow problems are considered.

In the fifth chapter, numerical studies of the efficiency of high-performance computing using hybrid parallel algorithms for airflow problems in a complex nasal region are considered.

In conclusion, the results of the dissertation work are presented.

Publications and approbation of results. The results of the research work were discussed at scientific seminars of the Department of Computer Science of al-Farabi KazNU and also were reported at international conferences. The results of the dissertation were published in 11 papers, 2 of them from the list, the THOMSON REUTERS database and 4 from the list, the SCOPUS database, 6 articles from the list recommended by the Committee for Control in Education and

Science of the Ministry of Education and Science of the Republic of Kazakhstan, 1 paper - in the materials international and republican conferences.

References:

1. Исахов А.А., Абылкасымова А.Б., Мансурова М.Е. Применение метода балансировки нагрузки на высокопараллельных вычислительных кластерных системах. Вестник КБТУ. – 2021, – № 1 (18) – С.117-125
2. Исахов А.А., Абылкасымова А. Исследование движения воздуха в респираторной системе человека методами математического моделирования. Известия КГТУ им. И. Раззакова. 2016, – № 3 (39) – С.116 – 121.
3. Исахов А.А., Абылкасымова А. Свойства переноса воздуха в респираторной системе человека с помощью численного моделирования. Вестник КазНУ. 2017. – № 1 (93) – С.105 – 118
4. Исахов А.А., Абылкасымова А., Сакыпбекова М. Применение параллельных вычислительных технологий для моделирования процесса отрыва течения за обратным уступом в канале с учетом сил плавучести. Вестник КазНУ. 2018. – № 1 (97) – С.143 – 158
5. Исахов А.А., Абылкасымова А. Применения параллельных вычислительных технологий для численного моделирования переноса воздуха в респираторной системе человека. Вестник КазНПУ, 2017, – № 1(57) – С.219-229.
6. Issakhov A.A., Zhandaulet Y., Abylkassymova A., Issakhov As. A numerical simulation of air flow in the human respiratory system for various environmental conditions. Theoretical Biology and Medical Modelling, 18, Article number: 2 (2021), doi.org/10.1186/s12976-020-00133-8 (2020 Impact Factor: 2.432, Q2; Scopus: SJR 2020 - 0.756, procentile - 71)
7. Issakhov A.A., Mardieyeva A., Zhandaulet Y., Abylkassymova A. Numerical study of air flow in the human respiratory system with rhinitis. Case Studies in Thermal Engineering Available online 19 May 2021, 101079, 10.1016/j.csite.2021.101079 (2020 Impact Factor: 4.724, Q1; Scopus: SJR 2020 - 0.913, procentile - 89)
8. Issakhov A., Abylkassymova A. Numerical study of identification of the main characteristics of air transport in the human nasal cavity. International journal of biology and biomedical engineering. Volume 11, 2017. P. 80-87 (SJR 2020 - 0.149 , procentile - 15)
9. Issakhov A.A., Abylkassymova A., Application of Parallel Computing Technologies for Numerical Simulation of Air Transport in the Human Nasal Cavity. Innovative Computing, Optimization and Its Applications. Studies in Computational Intelligence, vol 741. Springer, Cham. pp 131-149 In: Zelinka I., Vasant P., Duy V., Dao T. (eds) (SJR 2020 - 0.185, procentile - 24)
10. Issakhov A.A., Abylkassymova A., M. Sakypbekova Applications of parallel computing technologies for modeling of the wind flow around the architectural obstacles with the vertical buoyancy forces. Известие НАН РК, 2018 Серия физ.-мат. – № 4(320) – С.48-57

11. Issakhov A.A., Abylkassymova A., M. Sakypbekova Applications of parallel computing technologies for modeling the mixed convection in backward-facing step flows with the vertical buoyancy forces. International Journal of Mathematics and Physics, Volume 8. Number 2 (4). 2017. P. 43-50