

ABSTRACT

Author: Sarsembayev Magzhan Smagulovich

Specialty: 6D070400 – “Computer Engineering and Software”

Degree: Doctor of Philosophy (PhD)

Dissertation topic: “Development of High-Performance GPU Algorithms for Solving the Kinetic Equations of Combustion Processes”

General Description of the Work

The dissertation is aimed at creating a software package for accelerating computations in chemical kinetics problems.

Relevance of the Research Topic

Accurate modeling of combustion processes is an important scientific and technical task for energy, ecology, industrial safety, and the study of alternative fuels. The efficiency and environmental performance of systems such as internal combustion engines, gas turbine units, thermal power plants, and industrial combustion chambers directly depend on the accuracy of the combustion process description.

The combustion process is characterized by complex physicochemical phenomena, including chemical reactions, heat and mass transfer, gas dynamics, interaction of multicomponent mixtures, and formation of reaction products. To fully describe such processes, it is necessary to solve a system of differential equations of chemical kinetics. However, real combustion mechanisms consist of a large number of chemical components and reactions. Therefore, the calculation of kinetic equations requires significant computational resources and high-performance numerical algorithms.

Traditional CPU-based computational methods are not always sufficiently efficient for complex chemical kinetic systems. As the number of reactions increases, computation time grows significantly, which makes it difficult to model combustion processes using large mechanisms within a practically acceptable time. A particularly high computational load arises when modeling the combustion of multicomponent hydrocarbon fuels, the formation of harmful emissions, nitrogen oxides, and soot particles.

One of the effective ways to solve these problems is the optimization of chemical kinetic mechanisms and the use of specialized software tools that reduce computational costs. Such approaches make it possible to reduce complex mechanisms, efficiently process reaction systems, and accelerate numerical modeling.

In addition, the use of high-performance parallel computing technologies is an important direction in solving chemical kinetics equations. GPU architecture allows a large number of computational threads to be executed simultaneously, while in chemical kinetics problems many reaction-related operations can be performed independently of one another. Therefore, distributing such computations among GPU threads is an effective way to reduce calculation time.

Modern computational complexes and adaptive mesh methods describing reacting flows are also widely used for modeling combustion processes in high-

performance computing systems. Such approaches make it possible to describe complex combustion phenomena more accurately in spatial and temporal aspects.

Thus, the development of high-performance GPU algorithms for calculating kinetic equations of combustion processes is a relevant direction for modern scientific and applied problems.

An additional difficulty in solving kinetic equations is associated with the need to repeatedly evaluate the right-hand sides of the system at each time step of numerical integration. When detailed combustion mechanisms are used, each iteration includes the calculation of reaction rate constants, processing of stoichiometric coefficients, evaluation of the contributions of individual reactions to changes in component concentrations, and subsequent summation of these contributions. As a result, even a relatively small computation may require a large number of arithmetic operations, while for mechanisms containing hundreds of components and thousands of reactions, the computational load increases many times over.

Under these conditions, not only parallelization of computations but also the rational organization of GPU memory access becomes especially important. Efficient use of the GPU memory hierarchy, including global memory, shared memory, and registers, makes it possible to reduce data access latency and improve the performance of the computational kernel. Therefore, the development of GPU algorithms for chemical kinetics problems should take into account both the mathematical structure of the kinetic equations and the architectural features of CUDA devices, including the distribution of reactions among threads, synchronization of computations, and accumulation of reaction contributions to changes in component concentrations.

Aim of the Work

The aim of the work is to develop high-performance GPU algorithms for solving kinetic equations of combustion processes, implement them in software, and improve computational efficiency.

Research Objectives

- to analyze kinetic models of combustion processes and study numerical methods for solving them;
- to develop parallel algorithms adapted to GPU architecture;
- to implement the algorithms using CUDA, optimize memory usage and the computational process, and evaluate the accuracy and performance of the algorithms;
- to conduct a comparative analysis of CPU and GPU approaches.

Research Methods

The research used methods of chemical kinetics theory, mathematical modeling, numerical integration methods, the Runge–Kutta method, parallel computing methods, CUDA programming technology, GPU memory optimization techniques, comparative analysis of CPU and GPU computation times, and methods for evaluating the results of computational experiments.

Object of the Research

The object of the research is chemical kinetic mechanisms describing combustion processes and the system of kinetic equations formed on their basis.

Subject of the Research

The subject of the research is algorithms for parallel calculation of kinetic equations of combustion processes on GPU architecture, methods for software implementation of a CUDA-based kinetic solver, and approaches to efficient GPU memory organization.

Scientific Novelty of the Obtained Results

For the first time in combustion process modeling problems, a high-performance algorithm was developed for solving the system of equations of a chemical kinetic mechanism containing 162 components and 1006 reactions on GPU architecture. At the first stage of CUDA-based computations, a 17.5-fold acceleration was achieved compared with the CPU method. Subsequently, due to efficient GPU memory organization, the use of shared memory, and optimization of the computational process, the calculation speed for a complex mechanism containing 493 components and 2716 reactions was increased up to 154.89 times compared with the CPU method.

Provisions Submitted for Defense

The proposed GPU algorithms demonstrated a 17.5-fold acceleration compared with CPU-based methods at the initial stage, while optimization of GPU memory using shared memory increased the computation speed up to 154.89 times, confirming their high performance.

Theoretical and Practical Significance of the Research

The theoretical significance of the research lies in the fact that the obtained results contribute to the development of methods for parallel calculation of chemical kinetics equations on high-performance GPU architecture. The work considers the theoretical and algorithmic foundations of distributing a reaction system among CUDA threads, using the GPU memory hierarchy, and implementing the Runge–Kutta method in parallel.

The practical significance of the research is that the developed algorithms and software solutions make it possible to calculate complex combustion mechanisms in a short time. This approach can be applied in combustion process modeling, alternative fuel research, optimization of energy systems, assessment of harmful emissions, and high-performance scientific computing.

Scope and Structure of the Dissertation

The dissertation consists of an introduction, three sections, a conclusion, a list of references, and an appendix. The total volume of the dissertation is 123 pages. The work contains 43 figures, 3 tables, and 47 formulas. The list of references includes 74 sources.

Approbation of the Work

The results of the work were discussed at scientific seminars of the Department of Computer Science and the Faculty of Information Technology of Al-Farabi Kazakh National University, and were also presented at the following conferences:

- Sarsembayev M.S., Urmashev B.A. Development of a kinetic mechanism for methane combustion with the formation of nitrogen oxides and polyaromatic molecules // Proceedings of the International Conference “Innovative Development and Demand for Science in Modern Kazakhstan.” — Almaty, 2017.

- Sarsembayev M.S., Makashev E.P., Urmashev B.A., Isakhov A.A. Influence of supersonic flow temperature on diffusion combustion of hydrogen // Proceedings of the III International Conference “Industrial Technologies and Engineering.” — Shymkent, 2016.

- Sarsembayev M.S., Urmashev B.A. Creation of a kinetic mechanism for methane combustion with the formation of nitrogen oxides // Proceedings of the II International Scientific and Practical Conference “Modern Methodology of Science and Education.” — Warsaw, Poland, 2018.

Publications

Four printed works have been published on the topic of the dissertation, including 3 papers in publications recommended by the Committee for Quality Assurance in the Sphere of Science and Higher Education of the Republic of Kazakhstan, one paper in a peer-reviewed journal included in international citation databases Web of Science and/or Scopus, and three papers in proceedings of international conferences.

In addition, based on the results of the dissertation research, a copyright object was registered: **“Information and Computing System for the Automated Generation of Chemical Models Describing the Combustion of Real Fuels.”** Certificate No. 13255 on the entry of information into the State Register of Rights to Copyright-Protected Objects was issued on November 17, 2020, in the Republic of Kazakhstan (Appendix B).

Relationship of the Research with Scientific Projects

The dissertation was carried out within the framework of the following scientific projects:

- “Development of the theoretical foundations and prototype of a cloud-based information and computing system for the automatic generation of chemical models describing the combustion of real fuel” Research Project No. 0115RK00770, 2015–2017;

- “Creation and implementation of a cloud-based information and computing complex for the automatic development and optimization of pharmacokinetic and pharmacodynamic models” Project IRN: AP051329, 2018–2020.