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HIGH PERFORMANCE 3D SIMULATOR FOR LARGE EDDY SIMULATION OF TURBULENT REACTING FLOWS USING FILTERED DENSITY FUNCTION

ABSTRACT

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Relevance of the research. One of the most challenging issues in the field of energy and environmental research is related to the accurate prediction of turbulent reacting flows. Even in the days of Osborne Reynolds (over a century ago), there was a need to develop accurate methods for predicting the behavior of chemically inert and reactive turbulent flows.

One of the possible ways of classifying methods for calculating turbulent flows is based on the ratio of the "exactly" resolved and simulated parts of the turbulent energy spectrum. Based on these considerations, there are three main approaches to the numerical simulation of turbulent flows: (I) Direct numerical simulation (DNS), (II) Reynolds-averaged Navier-Stokes equations (RANS), (III) large eddy simulation (LES).

Direct numerical simulation (DNS) is a numerical solution of the full Navier-Stokes equations with physically consistent accuracy in space and time in such a way as to resolve all parts of the turbulence energy spectrum (i.e., describe the vortices of all scales). The step of integration over time and the size of the cells for spatial integration should be small enough to resolve all values of the Kolmogorov scale. Such requirements severely limit the range of tasks. Today, DNS calculations are carried out with a Reynolds number of about 10^5. For example, the Reynolds number of air flow around a car at a speed of 100 km / h is about 10^6, and the Reynolds number of atmospheric currents that determine the weather varies from 10^9 to 10^{11}. Thus, Thus, DNS allows simulating flows only with a small Reynolds number.

RANS is intended for statistical flow description. Time averaging is used to reduce the range of scales present in turbulent flows. The averaging time is much larger than the largest time scale of turbulent fluctuations, and the result is a conservation equation that describes the evolution of only the mean flux values. Flow quantities such as velocity and pressure are classified into mean and fluctuation components based on the Reynolds expansion. The influence of the measured turbulence fluctuations on the mean flow is included in the Reynolds stress tensor.

The disadvantage of the RANS is that no turbulence models obtained by RANS are perfect. When calculating certain flows, it is necessary not only to choose the most suitable turbulence model, but also to assess the degree of reliability of the results

obtained with its help. The main models of turbulence are based on the laws of simple "canonical" flows such as: the law of the wall, Kolmogorov's formula, etc. As soon as these patterns cease to be fulfilled, the calculation accuracy drops. Constants in turbulence models are “tuned” to a specific set of flows; each model has its own "scope". Also, the results obtained do not sufficiently cover the physics of flow.

A third approach, known as large eddy simulation (LES), in which instead of simulating all the turbulent quantities of flow, as is done in RANS, large eddies are solved directly and the smallest eddies of subgrid scale are simulated. Such modeling makes it possible to solve applied problems with high accuracy, and at the same time, the requirement for mesh resolution is much lower compared to direct numerical modeling (DNS). The LES is more accurate than the RANS approach as large eddies contain most of the turbulent energy and are responsible for most of the momentum transfer and turbulent mixing, and the LES captures these eddies in great detail directly while they are modeled in the RANS approach. In addition, small scales tend to be more isotropic and homogeneous than large ones, and thus modeling SGS motions should be easier than modeling all scales within a single model as in the RANS approach.

The successful implementation of LES depends on two factors: (1) how accurately the subgrid scale (SGS) quantities are modeled, (2) and how accurately these models are solved using numerical methods.

The filtered density function (FDF) methodology has proven to be most effective for closing the system of equations of LES. The main advantage of FDF is that after its application, the source of chemical reactions in the transfer equation of scalar variables is obtained in a closed form. Another important advantage is that closures of subgrid-scale quantities (for example, subgrid stress tensor, subgrid mass flow, etc.) using FDF are equivalent to second-order SGS models, while most current SGS models (for example, Smagorinsky model) have order zero, including dynamic versions.

In the LES method, a very desirable factor is that with increasing mesh resolution and / or increasing the order of accuracy of the applied scheme, the influence of the subgrid scale values decreases (striving for a DNS solution). It is also desirable that the prediction accuracy of the LES method does not depend on the grid cell sizes. The discontinuous Galerkin (DG) method in combination with the Monte Carlo method is able to satisfy all of these criteria.

Such a combination of mathematical and numerical modeling provides reliable prediction of turbulent flows. However, this approach is computationally demanding, especially for applications involving chemical kinetics. The reason for this is the huge number of particles in the Monte Carlo method, which is on the order of millions to billions of particles. For each particle, a system of stochastic differential equations is solved numerically. Even so, the LES method's requirement for resolving the computational grid is several orders of magnitude less than DNS.

The simulation time for applied problems using the proposed LES / FDF model using sequential code reaches order of months, sometimes might reach order of

several years. Therefore, the use of parallel technology is required. Parallel code can be adapted on computing systems based on a CPU (central processing unit) and / or on a GPU (graphics processing unit). It is known that the GPU has a number of advantages over the CPU. The main one is its cost. If you assemble a computing system based on a GPU, then its cost will be several orders of magnitude less than the cost of an equivalent in performance computing system based on a CPU.

In our work, we propose to develop a new highly efficient large eddy simulator of complex turbulent flows. To achieve high efficiency, the above mathematical model FDF, hybrid DG-MC scheme and high performance computing based on GPUs will be included in this software package. The results of the work will expand the capabilities of FDF, which will make it possible to solve more complex and applied problems in the field of studying reacting turbulent flows.

The aim of this dissertation work is to create a numerical methodology for large eddy simulation of reacting turbulent flows based on the filtered density function model using the discontinuous Galerkin method and high performance computing on GPUs. This approach makes it possible to reliably and efficiently solve a wide range of turbulent problems, including chemically reacting flows.

To achieve the aim, the following **research objectives** are formulated:

- To develop an incompressible flow solver based on the discontinuous Galerkin method. The Navier-Stokes equations averaged by the large eddy simulation approach.
- To develop a numerical methodology for the numerical solution of the modelled FDF transport equation using the particle based Lagrangian Monte Carlo method and integrate it with the main solver.
- Development and implementation of a parallel algorithm for the discontinuous Galerkin method using CUDA technology.
- Development and implementation of a parallel algorithm for the Monte Carlo method using CUDA technology.
- Analysis of the computational and overall performance of the developed numerical methodology by the means of large eddy simulation of a temporally developing two-dimensional and three-dimensional mixing layer under both non-reacting and reacting conditions.

The object of the research is turbulent reacting flows of an incompressible fluid.

The subject of the research is large eddy simulation of a temporally developing mixing layer based on the filtered density function model using discontinuous Galerkin numerics and high performance computing on GPUs.

Research methods: modern methods of mathematical and numerical modeling of dynamics and chemical kinetics of slow turbulent flows.

The scientific novelty is that that the DG-MC hybrid scheme for the numerical solution of the LES / FDF model was first developed and implemented using the CUDA technology for performing high performance computing on graphics

processing units. This significantly expands the range of problems available for numerical solution for researchers.

Scientific provisions for the defense:

A numerical methodology of numerical solution of the filtered incompressible Navier-Stokes equations based on the discontinuous Galerkin method using the filtered density function subgrid modeling;

- Development of a parallel algorithm for the discontinuous Galerkin method for solving basic flow equations using CUDA technology;
- Development of a parallel Monte Carlo algorithm for solving the transport equation of the filtered density function using CUDA technology;
- Analysis of the performance of the developed numerical by the means of large eddy simulation of a temporally developing two-dimensional and three-dimensional mixing layer.

The reliability and validity of scientific statements, conclusions and results of the dissertation work is determined by the use of fundamental conservation laws when constructing the mathematical models; satisfactory agreement of the simulated numerical results with the direct numerical simulation data.

Theoretical and practical significance of the results. The new numerical methodology of the filtered density function developed in the dissertation for large eddy simulation of reacting turbulent flows based on the discontinuous Galerkin method using the CUDA technology for parallel computations can be applied for further numerical investigation of two- and three-dimensional turbulent reacting flows, including theoretical and applied problems.

Links to other research work. This work was carried out within the framework of the project of the grant funding program for fundamental research in the field of natural sciences of the Ministry of Education and Science of the Republic of Kazakhstan " High Performance Discontinuous Galerkin–Monte Carlo Filtered Density Function 3D Simulator for Large Eddy Simulation of Reacting Turbulent Flows" (2018-2020, № ГР 0118РК00564).

Approbation of the work. The main provisions and results of the dissertation have been reported and discussed at the following scientific events:

- APS March Meeting 2017, Session V35: General Fluid Mechanics (March 13–17, 2017, New Orleans, Louisiana, USA);
- 70th Annual Meeting of the APS Division of Fluid Dynamics, Session M30: High Performance Computing (November 19–21, 2017; Denver, Colorado, USA);
- Актуальные проблемы информатики, механики и робототехники. Цифровые технологии в машиностроении (October 4-5, 2018, Almaty);
- Seventeenth International Conference on Numerical Combustion (May 6-8, 2019 Aachen, Germany);
- International scientific conference «Inverse Problems In Finance, Economics and Life Sciences» (August 31– September 4, 2019, Almaty);

- scientific seminars at the Laboratory for Computational Transport Phenomena, Department of Mechanical Engineering, University of Pittsburgh (2017, 2018, Pittsburgh, PA, USA);

- scientific seminars at the Department of Mechanics and Mathematics, Al-Farabi Kazakh National University (2014-2019, Almaty);

- scientific seminars at the Department of Applied Mechanics and engineering graphics, Satbayev University (2019, Almaty);

Publications. On the topic of the dissertation, the author has published 9 works, including1 article in a foreign scientific journal included in the Scopus and Web of Science databases with an impact factor of 1.071; 3 articles in journals recommended by the Committee for Control in Education and Science of the Ministry of Education and Science of the Republic of Kazakhstan; 3 abstracts published in the materials of foreign conferences; 2 theses in the materials of international conferences held in the Republic of Kazakhstan.

The structure and scope of the thesis. The dissertation work consists of an introduction, four chapters, a conclusion, a list of used sources of 74 works. The work is presented on 80 pages, contains 38 illustrations, 6 tables.

The introduction reflects the following points: relevance, main objectives of the work, novelty, scientific and practical significance of the dissertation work, the degree of its elaboration.

The first section is devoted to the mathematical model of the flow and contains two subsections. In the first subsection, the main filtered flow equations are derived based on the large eddy simulation approach and a closure strategy using the Smagorinsky method is described. The second subsection describes a method for closing chemical sources using a modelled filtered density function transport equation.

The second section is devoted to the numerics of the flow and contains four subsections. In the first subsection, we give a general formulation of the discontinuous Galerkin method for the conservation equation in a weak form using Legendre basis functions. In the second and third subsections, the time discretization of the basic equations using the Chorin's projection method and the spatial discretization of the basic flow equations using the discontinuous Galerkin method are presented, respectively. The fourth subsection reflects a numerical algorithm for solving the transport equation of the filtered density function using the Lagrangian Monte Carlo method.

The third section is devoted to the parallel implementation of the numerical methodology using GPUs and contains two subsections. In the first subsection, a parallel algorithm of the discontinuous Galerkin method using the CUDA technology is developed. It describes the optimal use of each memory type and determines the most appropriate thread block size. In the second subsection, a parallel Monte Carlo algorithm is developed using CUDA technology. It reflects the detailed implementation of each of the five stages, including the choice of the random number

generation algorithm, the distribution of threads in the block and the optimal use of the device memory.

The fourth section presents the flow parameters. As a test problem, large eddy simulation of a temporally developing mixing layer under both non-reacting and reacting conditions is considered. The problem is simulated in 2D and 3D spaces. Physical parameters are given, including the Reynolds number and the Damkeler number; and numerical parameters, including mesh resolution and order of the Legendre polynomial.

The fifth section reflects the results of calculations and contains two subsections. In the first subsection, results are presented regarding the computational performance of the developed numerical methodology. For the two-dimensional case, the performance is estimated by comparing the calculation results obtained using a parallel algorithm on a graphics device with the calculation results obtained by sequential calculations on the central processor. Scalibility of the solver in 3D calculations is estimated by determining the number of floating point operations per second. The second subsection presents the results regarding the predictive capabilities, consistency and convergence of the developed LES-FDF-DG hybrid scheme. The consistency and convergence of the scheme is assessed by comparing the solutions of the first and second moments of scalars obtained using FDF and DG calculations. The results obtained are analyzed statistically by calculating the Reynolds-averaged SGS stresses, resolved stresses and total stresses. The results are given taking into account the chemical reaction for different Damkeler numbers.

In the conclusion, the main results and conclusions obtained in the dissertation work are presented.