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USING THE CUDA TECHNOLOGY TO SPEED UP COMPUTATIONS IN PROBLEMS OF CHEMICAL KINETICS

Abstract. The main idea of the implementation is reducing the time for calculation and thereby implement a multi-user mode for users by placing it on a server with access via a web browser. To model the kinetics of chemical reacting systems were used 4th and 5th grade Runge-Kutta methods and to receive the index of advantages of this elaboration were written programs in C# for sequential computation on a central processor and was used a platform for parallel computation of CUDA on graphic processors. Parallelization of data during calculation on a GPU was performed by the distribution of the reaction to individual strands, when changes of the concentration was calculated over a given time interval of a certain substance. Parallelization is performed over all elementary reactions, with the increasing of the number of reactions in the mechanism, because of this the computation on the GPU has a noticeable gain in time.

Keywords: CUDA, combustion, modeling, parallel computation, performance, computing, thermodynamics, concentration changes, reactions of mechanism.

Nowadays computing technologies significantly permits to increase the speed of mathematical modeling of any processes. However not all program complexes efficiently allows to use parallel processing of the received data. In this case, it concerns to parallel computing with using graphics processors [1-3].

The purpose of the work is to use an NVIDIA graphics card with the calculative abilities of the graphic processors for acceleration of definite chemical reactions processing under different temperature regimes. There was condacted a comparative analysis of programming technologies using graphic processors is carried out. After analyzing of their features and capabilities, the CUDA (Compute Unified Device Architecture) technology, which was developed by NVIDIA, was chosen as the most convenient in terms of programming and presented features. CUDA is a parallel computing architecture from NVIDIA, which significantly allows you to increase computing productivity due to using the GPUs (graphics processors). The applying of this a parallelization technology for solving the equations of chemical kinetics makes it possible to reduce the time and computational costs [4-10].

CUDA computing flows are performed on a separate physical device, the so-called device, which is used as a central processor's (CPU) coprocessor. In its turn, the program in CUDA-C language, the so-called kernel, starts from the central processor for each of the computational flows. The threads' configuration is set on the CPU before the kernel function's calling. For convenience and best performance, computational flows are combined into blocks, which then are combined into a grid. In the course of the implementation of then massively parallel kinetic solver was developed the "Chemical Calculator" software for simulating the kinetics of chemically reacting systems at the zero-dimensional approximation. The work of the program combines the process of computing, the central processing unit and the NVIDIA graphics processor, using CUDA technologies [11-14].

The graphical interface of the program was developed with the use of C # language [2-5]. The program interface was created in the maximally convenient way for users at solving problems of chemically reacting systems. The type of software is shown in figure 1.

Abbreviated files of the Chemkin mechanismare are used at the performing of calculations in the developed program. It allows the user to easily transfer their bulk mechanisms into the Chemkin format [2; 4; 6]. The user can download these files using the menu items File → Reactions and File → Thermodynamic Properties. After downloading, the input files appear in the "Input file" program area. Here the separator between the reactions and the thermodynamic properties of substances is a string, which contains the word "THERM". Reading data from the "Input file" area is done line by line and the results of reading are written at the "Reading results" area. The number of reagents and reactions in a given mechanism, the Arrhenius formula coefficients, the direction of the reaction, the derivation of the left and right matrix for the reaction mechanism and the thermodynamic data for each element in the mechanism are determined as a result of reading. The definition of this data is made with only one click of the menu item Reading → Reading the data from a file. After this the input data is entered for conducting calculations, choosing a certain method from the drop-down list. Calculations can be conducted on the central processor as well as on the GPU [6; 10]. At performing of the calculations on NVIDIA with an increasing of the number of computations, time of calculations decreases in comparison with computing time on central processors [11-14].

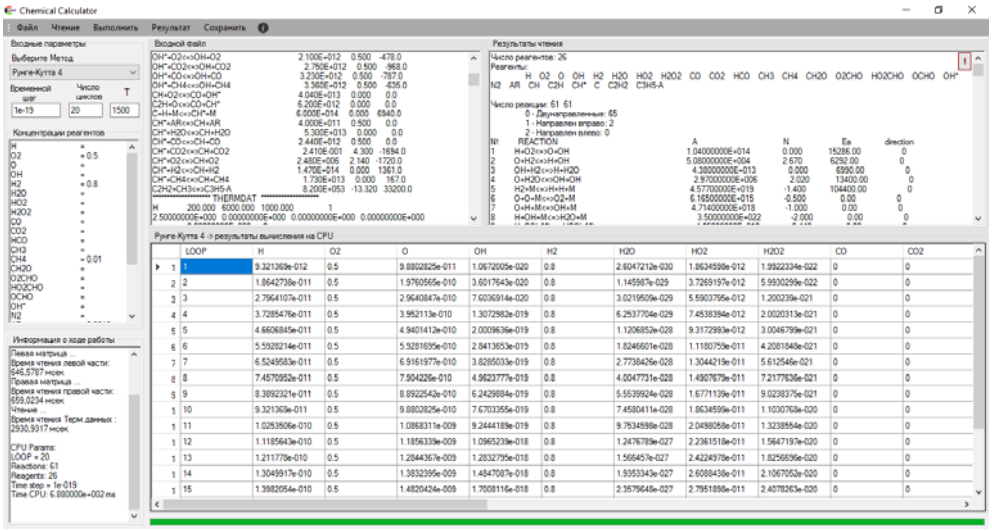

Figure 1 - The main interface of the program "Chemical calculator"

To simulate the kinetics of chemical reacting systems used of grade Runge-Kutta methods. This methods was written a C # program code for sequential computation on the central processor and CUDA technology was used for parallel computation [14-17].

Table 1 - Comparative analysis of the estimated time in the CPU and GPU for different sizes of the input mechanism

Mechanism: Aramco_Mech				
4th grade of Runge-Kutta methhod				
Number of chemical elements	Number of chemical reactions	Regime of calculations of CPU, msec	Regime of calculation of GPU, msec	Received accelerationx10
21	51	6901,00	9080,24	0,76
33	118	39081,00	20204,50	1,93
39	191	87735,00	29619,10	2,96
52	245	199169,00	49747,80	4,00
61	301	336749,00	67557,10	4,98
66	376	491811,00	83188,70	5,91
84	448	946439,00	125339,00	7,55
103	565	1795548,00	186175,00	9,64
162	1006	6832052,80	390403,00	17,5

In table 1 is given comparative analysis of CPU and GPU time of calculation. Parallelization of data during the calculation for the GPU is carried out by distributing the reactions on separate strings, at the calculating changes of concentrations in a given time interval of a certain substance [15; 18; 19-28].

Each thread calculates how much the concentration of a given substance in a definite reaction has changed over a cerain time interval.Parallelization is performed by reactions with increasing of the number of reactions in the mechanism, that's why computation on the GPU considerably saves time (table 1).

The program implements automated reading of data from input files to the Chemkin software package format, subtracted algorithms for calculating rates of reactions, calculating changes in the concentration of substances over time [25-28]. The main calculations could be performed by 4th grade of Runge-Kutta method [29]. The computation on the central processor is performed by using a sequential algorithm. Calculation on NVIDIA graphics cards, using CUDA parallelization technologies, is performed in parallel way. The use of enterprise software was made by a comparative analysis of the computation time on the central processing unit and on the graphics processor. As a result, it was found that accelerating of the computation process using graphics cards gives a very good time win [27-29].

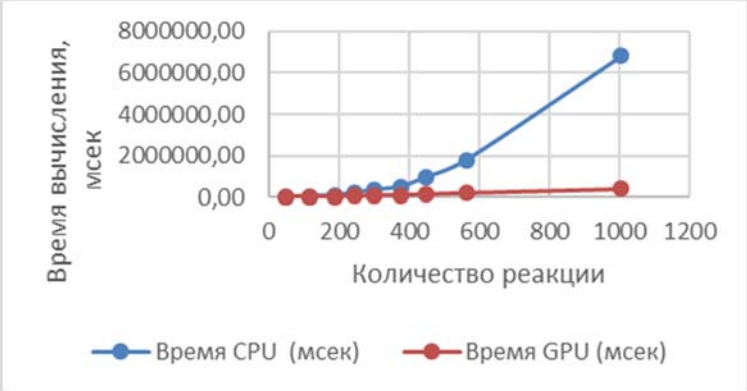

Figure 2 - Comparative analysis of computational algorithms on CPU and GPU using The fourth-order Runge-Kutta method

User's manual of the program "Chemical calculator". When you start the program, opens the main interface. The program interface consists of several components. In the upper area of the interface is a row of menu components. Loading of input files into the program is conducted through the menu item File. File - Thermodynamic properties (figure 2). These downloaded files are imported into the "Input file" program area. "Thermodynamic properties" - the program for automatic insertion of the word-separator "THERMDAT". During the reading of data from the "Input file" area, the beginning of the thermodynamic data line is determined from this word. If necessary, you can edit the input data of the mechanism directly in this area [25-29].

Reading of data from the input area is performed by clicking the menu item Read → Read data from the file . After clicking this menu item on the created algorithm of data recognition from the input area realizes the automatically reading of the data. At reading the data of reaction, four parameters are determined for calculating there action rates (formulas 1, 2).

The rate of the reverse reaction is determined by the following formula

$$k_{ri} = \frac{k_{fi}}{K_{c_i}} \tag{1}$$

$$K_{c_i} = K_{p_i} \left(\frac{P_{atm}}{RT}\right)^{\sum_{k=1}^{K} \nu_{ki}} \tag{2}$$

The first parameter is the pre-exponential factor, the second parameter is the temperature exponent, the third parameter is the energy activation and the fourth parameter determines the direction of reaction. If the reaction proceeds only in one direction, then only the rate of reaction is calculated only in this direction, in the other case it depends on the rate of the forward and reverse reactions. After reading these reactions, from reactions they all correspond to the reagents of this mechanism [23-29].

The left and right data matrix is then determined. In these matrices the corresponding coefficients of the elements in the given reaction are located. These data are also used at determining in rates of reaction(formulas 3, 4).

The rate of formation of the k-th substance (ω_k)˙ is calculated by the following formula [25-29]:

$$\dot{\omega_k} = \sum_{i=1}^{I} v_{ki}\, q_i \ (k = 1, \dots, K) \tag{3}$$

Here $v_{ki} = v''_{ki} - v'_{ki}$.

Rate of reaction progress' changing of *i*-reaction determines by following formula:

$$q_i = k_{fi} \prod_{k=1}^{K} [X_k]^{v''_{ki}} - k_{ri} \prod_{k=1}^{K} [X_k]^{v'_{ki}} \tag{4}$$

$[X_k]$ – the molar concentration of the *k*-substance, k_{fi} *and* k_{ri} the rate of direct and reverse reactions.

The rate of the direct reaction is determined by the Arrhenius form

$$k_{fi} = A_i T^{\beta_i} \exp\left(\frac{-E_i}{R_c T}\right) \tag{5}$$

Where R is the universal gas constant; A_i is a pre-exponential factor that does not depend on temperature, but is determined only by the type of reaction; B_i is the temperature exponent, E_i is the activation energy of the i-th reaction, which can be characterized as a certain threshold energy: roughly speaking, if the energy of the colliding particles is smaller, then the collision will not occur if the energy exceeds E_i. The activation energy does not depend on temperature.

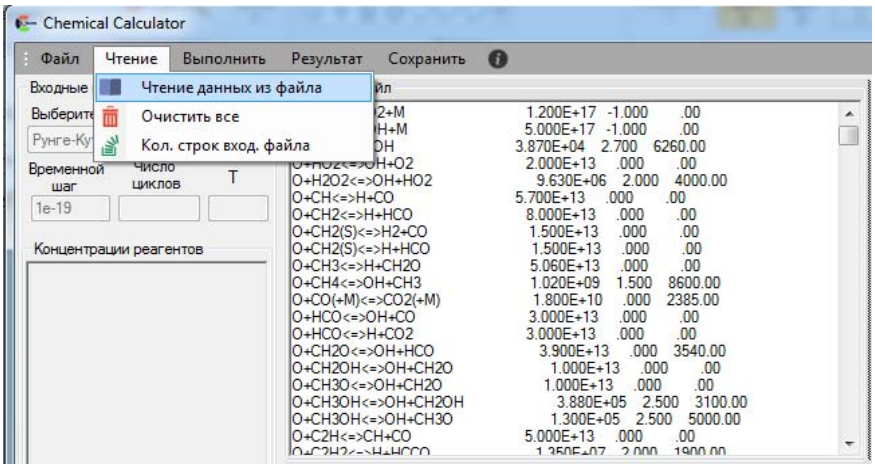

Figure 3 - Reading data from a file

Thermodynamic properties are read for each reagent of this mechanism from the input data of thermodynamic properties. Thermodynamic properties are determined by the heat capacity, enthalpy, entropy, free energies of Gibbs and Helmholtz, for a given substance (formulas 1-5) [28,29].

Basic equations of energy conservation in a medium with constant pressure

$$\frac{dT}{dt} = -\frac{1}{\rho \bar{c}_p} \sum_{k=1}^{K} H_k\, \dot{\omega}_k \tag{6}$$

Here, T is the temperature of the medium, ρ is the mass density, $\bar{c}_p$ is the specific heat, H_k is the molar enthalpy of substances and $\dot{\omega}_k$ is the velocity.

The thermodynamic properties of substances in standard states are temperature "ideal", therefore these properties are defined as temperature-dependent functions and at a constant pressure the heat capacity of these substances is written as a function depending on polynomial coefficients and temperature:

$$\frac{C^0_{pk}}{R} = \sum_{n=1}^{N} a_{nk} T_k^{(n-1)} \tag{7}$$

Here the sign of the superscript "0" denotes the properties of certain substance in 1 atm. pressure. For ideal gases the heat capacity is independent of temperature, so the value of the heat capacity in the standard state is relevant for them. Other thermodynamic properties of substances at a given temperature are determined in the form of integral functions depending on the specific heat.

The molar enthalpy of substances in standard states is determined by the following formula:

$$H_k^0 = \int_{298}^{T_k} C_{pk}^0 dT + H_k^0(298) \tag{8}$$

$$\frac{H_k^0}{RT_k} = \sum_{n=1}^{N} \frac{a_{nk} T_k^{(n-1)}}{n} + \frac{a_{N+1,k}}{T_k} \tag{8.1}$$

here, parametre $a_{N+1,k} * R$ denotes the heat of formation at 298K.

The molar entropy in the standard state is written in the form

$$S_k^0 = \int_{298}^{T_k} \frac{C_{pk}^0}{T} dT + S_k^0(298) \tag{9}$$

$$\frac{S_k^0}{R} = a_{1k} \ln T_k + \sum_{n=2}^{N} \frac{a_{nk} T_k^{(n-1)}}{(n-1)} + a_{N+2,k} \tag{9.1}$$

here, the constant of integration $a_{N+2,k} * R$ is determined depending on the value of the entropy of a given substance at a temperature of 298 K.

The equatations, which are given above, are indicated for polynomial of the permissible limits, used in the NASA chemical equations (formula 8). In the Chemkin software complex, these components are divided into two groups for two intervals of the temperature interval (low and high temperature region). In this case, to process the thermodynamic properties [11-14]:

$$\frac{C_{pk}^0}{R} = a_{1k} + a_{2k} T_k + a_{3k} T_k^2 + a_{4k} T_k^3 + a_{5k} T_k^4 \tag{10}$$

$$\frac{H_k^0}{RT_k} = a_{1k} + \frac{a_{2k}}{2} T_k + \frac{a_{3k}}{3} T_k^2 + \frac{a_{4k}}{4} T_k^3 + \frac{a_{5k}}{5} T_k^4 + \frac{a_{6k}}{6} \tag{11}$$

$$\frac{S_k^0}{R} = a_{1k} \ln(T_k) + a_{2k} T_k + \frac{a_{3k}}{2} T_k^2 + \frac{a_{4k}}{3} T_k^3 + \frac{a_{5k}}{4} T_k^4 + a_{7k} \tag{12}$$

Other thermodynamic properties have values C_p^0, H^0 и S^0. Specific heat at constant volume -C_{vk}^0

$$C_{vk}^0 = C_{pk}^0 - R \tag{13}$$

Interior energy U_k^0

$$U_k^0 = H_k^0 - RT \tag{14}$$

Gibb's free energy in a standard state G_k^0

$$G_k^0 = H_k^0 - T_k S_k^0 \tag{15}$$

Helmholtz free energy in the standard state A_k^0

$$A_k^0 = U_k^0 - T_k S_k^0 \tag{16}$$

For ideal gases in the standard state, the internal heat capacity, enthalpy and specific heat are equal to the actual value of these properties.

Equations for determining the reaction's rate

$$\sum_{k=1}^{K} v'_{ki} \chi_k \Leftrightarrow \sum_{k=1}^{K} v''_{ki} \chi_k \ (i = 1, \dots, I) \tag{17}$$

Stoichiometric coefficients v_{ki} integers and χ_k chemical symbol of k −substance. v'_{ki} − direct reaction's rate, v''_{ki} −reverse reaction's rate. Usually, three or four substances participate in elementary reactions.

To calculate the reaction rates in the "input data" area is set the initial temperature of the mixture and by clicking on the menu item **Run → Calculate velocities**, for each reaction, the rates of the forward and reverse reaction are calculated.

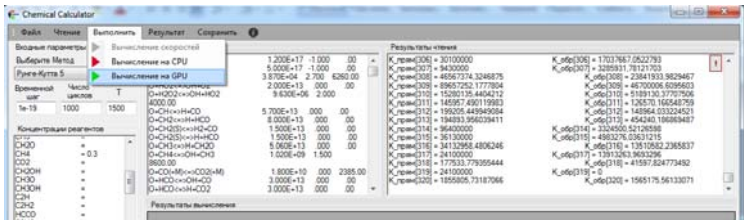

Figure 4 - Running the calculation on the GPU

In this program, the basic computational work can be done with the use of a sequential algorithm on the central processor as well as with the use of parallel algorithm in the graphics processor. Before calculating is chosen a method for calculating the change in concentration over time. Then, the time step and the number of cycles are set. The total calculation time is determined as follows:

$$t = Time\ step\ \times Number\ of cycles$$

As it can be seen from the input data, to calculate the change of concentration of all elements of this mechanism a sufficiently resource-intensive calculation is required. With a sufficiently large volume of the computation mechanism, using a sequential algorithm requires a lot of computational costs and time. And the use of a parallel algorithm makes it possible to speed up the computation with increasing the volume of the mechanism [2; 4; 11-14].

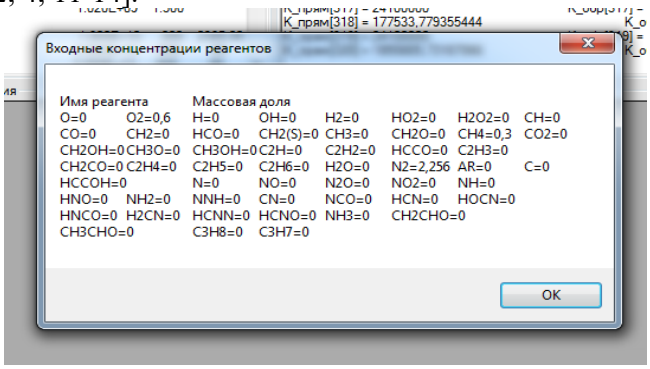

Figure 5 - Checking the concentration value before starting the calculation

For further calculation, the initial concentration of reagents in the mechanism is given in the "Concentration of substances" area. If the initial concentration for some substances is not specified, the initial concentration for these reagents is taken as zero (figure 5). After the end the calculation results are displayed in the form of a table (figure 6). For clarity, you can see this data in the form of a graph (figure 7). To do this, just choose.

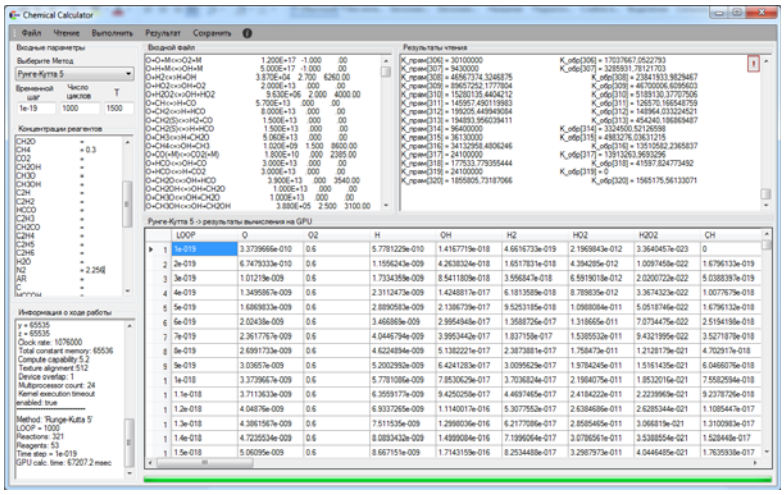

Figure 6 - Results of calculation

menu item **Result → Show res. GPU / CPU → Show in the graph.** After that, a separate window opens with the graphics area and in the right-hand area of the names of the reagent's mechanism and a label. At the inserting / removing a check mark in these marks a graph concentration changes of the substance over time appears in the graph area [17; 22; 24-27].

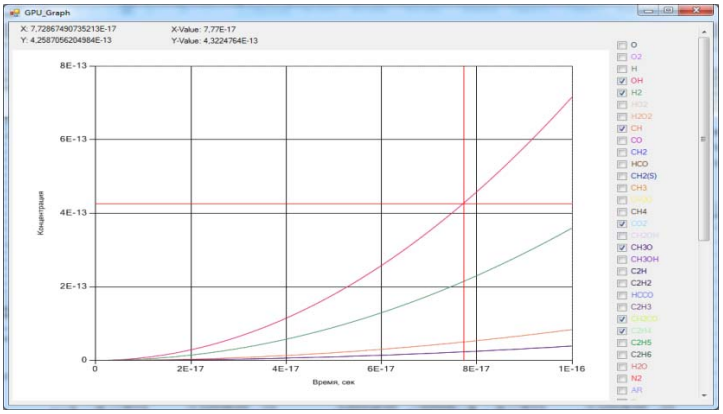

Figure 7 - Change in the concentration of substances by time

This technology and the calculation approach allowed to achieve acceleration by more than 17.5 times in comparison with multi-valued calculation on an IntelCore i7 3.4 GHz processor and 2-3 times in comparison with the best performance of a multithreaded version based on GCD technology on 2x IntelXeon processors 3.06 GHz with 24 cores. The results are obtained for loading parameters, which present practical interest in systems.

Conclusion. In the developed program are used abbreviated files of the Chemkin mechanism. It's allows to use in the created project their volumetric mechanisms in the format of the Chemkin software package. Calculations of the concentration of chemicals can be carried out both on the central processor and on the graphic one. When performing calculations on NVIDIA GPUs, with an increase in the number of chemical reactions, the calculation time decreases compared to the calculation time on central processors. The program implements modules for automated data reading from input files in the format of the Chemkin software package, computational algorithms for calculating reaction rates, and calculating changes in the concentration of substances over time. Basic calculations can be performed using the 4th and 5th order Runge – Kutta methods. The computation on the central processor is performed using a sequential algorithm. Computing on NVIDIA graphics cards, using CUDA parallelization technologies, is performed in a parallel type. Using the software gets a comparative analysis of the time interval of calculations on the central processor, as well as on the graphics processor, was carried out. As a result, when using the Aramco_Mech mechanism with the number of elements of 162 and with the reaction of 1006, it was found that the acceleration of the computation process using graphic cards can reduce the time by 17.5 times compared to the central processor.

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ХИМИЯЛЫҚ КИНЕТИКАНЫҢ МӘСЕЛЕЛЕРІНДЕ ЕСЕПТЕРДІ ЖЕДЕЛДЕТУ ҮШІН CUDA ТЕХНОЛОГИЯСЫН ПАЙДАЛАНУ

Аннотация. Іске асырудың негізгі идеясы - есептеу уақытын қысқарту және осылайша пайдаланушыларға арналған көп қолданушы режимін енгізіп, оны веб-сервер арқылы қолжетімділігі бар серверге орналастыру. Химиялық реакция жүйелерінің кинетикасын модельдеу үшін Рунге-Куттың 4-ші және 5-ші дәрежелі әдістері қолданылды. Осы әдістерді қолданып C# тіліндегі программалық код жазылды. Ол код

орталық процессорда тізбекті түрде есептеледі және параллельді есептеу үшін CUDA графикалық процессорларда параллельді есептеу платформасы қолданылды. Берілген уақыт аралығында белгілі заттың концентрациясының өзгеруін GPU-да деректерді параллельді есептеу үшін реакцияларды бөлек бағыттарға бөледі. Әр бағыт берілген уақыт аралығында белгілі заттың концентрациясы осы реакцияларда бөлінуі әр бағытта есептеледі. Параллельдеу барлық қарапайым реакциялар үшін жасалғандықтан,, механизмдегі реакциялар санының артуымен GPU есептеу уақытты әлде-қайда ұтымды етуге алып келеді.

Түйін сөздер: CUDA, жану, модельдеу, параллельді есептеу, өнімділік, есептеу, термодинамика, концентрацияның өзгеруі, механизм реакциялары.

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ПРИМЕНЕНИЕ ТЕХНОЛОГИИ CUDA ДЛЯ УСКОРЕНИЯ ПРОБЛЕМ ХИМИЧЕСКОЙ КИНЕТИКИ

Аннотация. Основная идея реализации - сократить время вычислений и тем самым реализовать многопользовательский режим для пользователей, разместив его на сервере с доступом через веб-браузер. Для моделирования кинетики химических реагирующих систем использованы методы Рунге – Кутта 4–го и 5–го порядка. С помощью этих методов было написано код программы на языке C# для последовательного вычисления на центральном процессоре и использовано платформа для параллельного вычисления CUDA на графических процессорах. Распараллелирования данных при расчете на GPU производится распределением реакции на отдельные нити, при вычислении изменений концентрации на заданном временном интервале определенного вещества. Каждая нить вычисляет, насколько изменилась концентрация данного вещества в данной реакции на заданном временном интервале. Так как распараллелирование производится по всем элементарным реакциям, с увеличением количеств реакций в механизме вычисление на GPU дает заметный выигрыш по времени.

Ключевые слова: CUDA, горение, моделирование, параллельные вычисления, производительность, вычисления, термодинамика, изменения концентрации, реакции механизма.

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