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# Mathematical Modeling of Detonation Initiation in the Channel with a Profiled End Using Parallel Computations

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The paper is devoted to a numerical study of detonation initiation in the gas mixture in the channel with a profiled end. Initiation occurs as a result of the reflection of the shock wave of relatively low intensity from the end of the channel. Numerical calculations are carried out using unstructured triangular grids. The numerical algorithm is parallelized by the computational domain decomposition method using the METIS library. The exchange of grid function values between computing cores is performed using the MPI library. Numerical calculations are conducted on grids with different numbers of triangular cells. Detonation initiation patterns are obtained, which correspond to each other. The differences are mainly related to the degree of resolution of the elements of the gas mixture flow in the channel.

*Keywords: detonation initiation, unstructured triangular grids, parallel computations, Kelvin–Helmholtz instability.*

## Introduction

Mathematical modeling of gasdynamic processes with chemical reactions, shock waves (SWs) and detonation waves (DWs) is of great interest from the point of view of fundamental and applied sciences. Scales of physical quantities and chemical reactions can significantly vary in space during the study of the process. In addition, gasdynamic processes with DWs have a complex nonlinear nature (see, for example, [1]), the comprehensive research of which in experiments is often associated with some difficulties. One of such problems is the study of the process of suppression of DWs that occur in tunnels and mines. Another, quite important on an industrial field, is the problem of creating a detonation engine based on rotating detonation in an annular channel. The issues of detonation initiation in channels are also of interest.

In this work, the initiation of a DW in a gas mixture under reflection of a SW from the curved end of the channel is considered. The SW propagation along the channel is accompanied by its interaction with the channel walls with the formation of new waves. The interaction of waves with each other and with the channel walls leads to the formation of so-called hot spots that are regions of high pressure and temperature (see, for example, [2]). In this case, hot spots become initiators of the mixture.

The problems noted above show that the study of the processes of initiation, propagation, and suppression of DWs can be carried out in a domain of complex geometry and with curved boundaries. In such cases, the domain is typically discretized using unstructured grids. Indeed, as noted in [3], it is impossible to generate automatically block-structured grids on arbitrary geometries. However, calculations on unstructured grids with a large number of cells are usually quite demanding on computer resources. One of the solutions is the use of parallel computational technologies, which makes it possible to carry out calculations in various studies in adequate periods of time.

The aim of the work is mathematical modeling of detonation initiation as a result of shock wave reflection from the profiled end of the channel using parallel computations.

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The article is organized as follows. Section 1 provides the statement of the problem and the mathematical model. Section 2 is devoted to the description of the numerical algorithm. Section 3 contains the results obtained in the calculations. Conclusion summarizes the study.

## 1. Problem Statement and Mathematical Model

The plane channel with the end consisting of three sections of a plane wall and two semi-ellipses arranged symmetrically relative to the axis of the channel is considered. The channel is filled with a model hydrogen-oxygen mixture. The pressure in the channel is 0.04 atm, the temperature is 298 K. The plane SW with a Mach number of 2.5 propagates towards the end of the channel. Taking into account the problem statement and the symmetry of the channel, we consider half of the channel to reduce the number of calculations. The geometry of the computational domain, as well as the boundary conditions, are shown in Fig. 1. Note that the geometry and the statement correspond to the data from the experimental work [1].

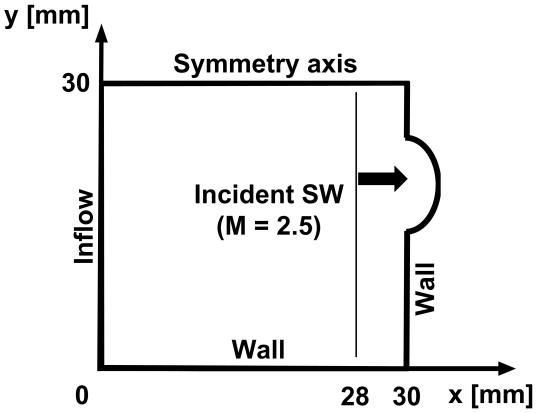



**Figure 1.** Schematic of the computational domain

The mathematical model is based on the 2D Euler equations written in the Cartesian frame $(x, y)$ and supplemented by one-stage chemical kinetics model. The system of governing equations has the following view:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \mathbf{S},$$

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \\ \rho Z \end{bmatrix}, \mathbf{F} = \begin{bmatrix} \rho u \\ p + \rho u^2 \\ \rho uv \\ (p+e)u \\ \rho Z u \end{bmatrix}, \mathbf{G} = \begin{bmatrix} \rho v \\ \rho uv \\ p + \rho v^2 \\ (p+e)v \\ \rho Z v \end{bmatrix}, \mathbf{S} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \rho\omega \end{bmatrix}, \tag{1}$$

$$e = \frac{\rho}{2}(u^2 + v^2) + \rho\varepsilon,\ \varepsilon = \frac{p}{\rho(\gamma - 1)} + ZQ,\ p = \frac{\rho}{\mu}RT,\ \omega = -A\rho Z exp\left(-\frac{E}{RT}\right).$$

Here, $t$ is the time, $\rho$ is the density of the gas mixture, $u$ and $v$ are the components of the gas velocity, $p$ is the pressure, $T$ is the temperature, $e$ is the total energy per unit the unit of the volume, $Z$ is the mass fracture of the reactive component of the mixture, $\omega$ is the rate of the chemical reaction, $\varepsilon$ is the specific internal energy of the gas, $Q$ is the heat release of the chemical reaction, $\mu$ is the molar mass of the gas, $R$ is the universal gas constant, $A$ is the pre-exponent

factor. The gas is considered to be ideal with the constant specific heat ration $\gamma$. The following values of the parameters are used:

$$\gamma = 1.23,\ \mu = 12\ \frac{\text{g}}{\text{mole}},\ Q = 7.37\ \frac{\text{MJ}}{\text{kg}},\ E = 76.2\ \frac{\text{kJ}}{\text{mole}},\ A = 9.16 \times 10^8\ \frac{\text{m}^3}{\text{kg s}}.$$

The parameters $\gamma$, $Q$, $E$ and $A$ are taken from the database [4]. The parameter values correspond to a pressure of 0.2 atm, which is equal to the pressure behind the SW reflected from the plane wall for the considered Mach number value and the initial pressure value of 0.04 atm.

## 2. Numerical Algorithm

The main feature of the computational technique is the use of completely unstructured numerical grids with triangular cells. A Delaunay triangulation is carried out to construct the grids. The computational algorithm is based on the technique of splitting physical processes. First, the gasdynamic equations are integrated on a time step. Then, the chemical kinetics equations are integrated on the time step using parameters obtained on the previous stage and not taking into account the effect of convection. On the gasdynamic stage, spatial discretization is conducted using the finite volume method. The numerical flux is calculated using the AUSM scheme. The reconstruction of grid functions with limiter minmod is applied. The numerical method employs a large stencil on triangular grids suitable for the second order of the accuracy. Time integration is carried out using a second order explicit Runge–Kutta scheme with two stages. On the second stage the system of 2 ordinary differential equations is solved numerically to find the values of gas temperature and mass fracture of the gas reactive component. The serial computational algorithm is described in more detail in [5].

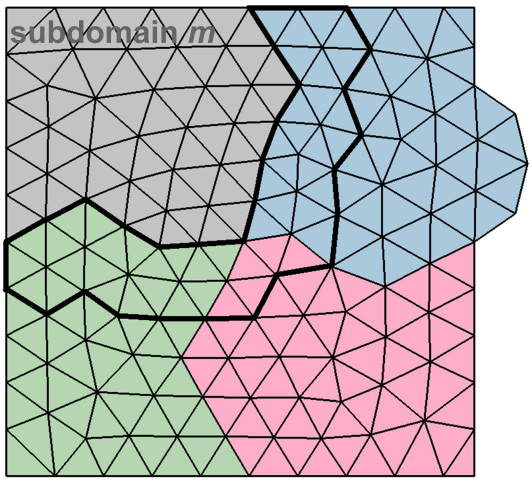



**Figure 2.** Example of decomposition of the computational domain into 4 subdomains. The bold line indicates the boundary of the halo-cells corresponding to the subdomain $m$

The computational algorithm is parallelized by the method of numerical grid decomposition. The realization of the parallel algorithm is carried out using the Message Passing Interface (MPI) technology. The computational domain is divided into subdomains using the METIS library. The number of subdomains is equal to the number of computing cores used in the computations. Thus, the computing core with the number $m$ corresponds to the values of gasdynamic parameters in cells from the subdomain $m$, as well as the values of the parameters in the halo-cells [6] of the subdomain m. An example of the decomposition of the computational domain

into 4 subdomains is shown in Fig. 2. The bold line indicates the boundary of the halo-cells corresponding to the subdomain $m$. The set of halo cells for each subdomain is determined by the location of the boundaries of the subdomains and the algorithm of gasdynamic parameters calculation. At each time step, parameter values in halo-cells are exchanged between computing cores. The exchange of values is carried out using standard methods of the MPI library. The MPI_Send and MPI_Recv blocking functions are quite effective in cases of such decompositions when a subdomain has one or two adjacent subdomains. In this work, the number of adjacent subdomains can be more than two, as shown in Fig. 2. So, we use the MPI_Alltoallv function that sends data from all to all computing cores. Then, the calculation of gasdynamic parameters in each subdomain is carried out using the actual values of the parameters in halo-cells. The computations are performed on the supercomputer MVS-10P (Joint Supercomputer Center of RAS).

During the computations, the distributions of gasdynamic parameters in the subdomain $m$ are periodically written to a CGNS file with a name corresponding to the computing core with the number $m$. Visualization of the spatial distributions of gasdynamic flow parameters is carried out using the open source tool Visit based on the Visualization ToolKit (VTK) library.

## 3. Results

A series of calculations of the detonation problem for a fixed numerical grid and a different number of computing cores is carried out. The numerical grid consists of 6 mln cells. The dependence of the parallel speedup on the number of cores is shown in Fig. 3. The deviation of the obtained dependence from the linear one is due to the following fact. The greater the number of computing cores, the greater the number of halo-cells. Moreover, in the case of a multidimensional computational domain, the number of halo-cells for various cores can be different. Thus, an increase in the number of cores can lead to the fact that the percentage of time associated with data exchange between cores will grow, and the percentage of time associated with calculations will fall due to a decrease in the number of triangular cells per core.

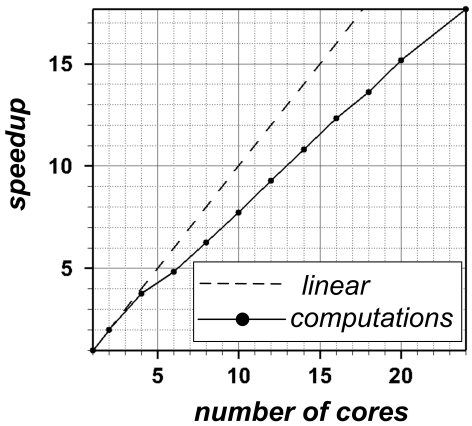
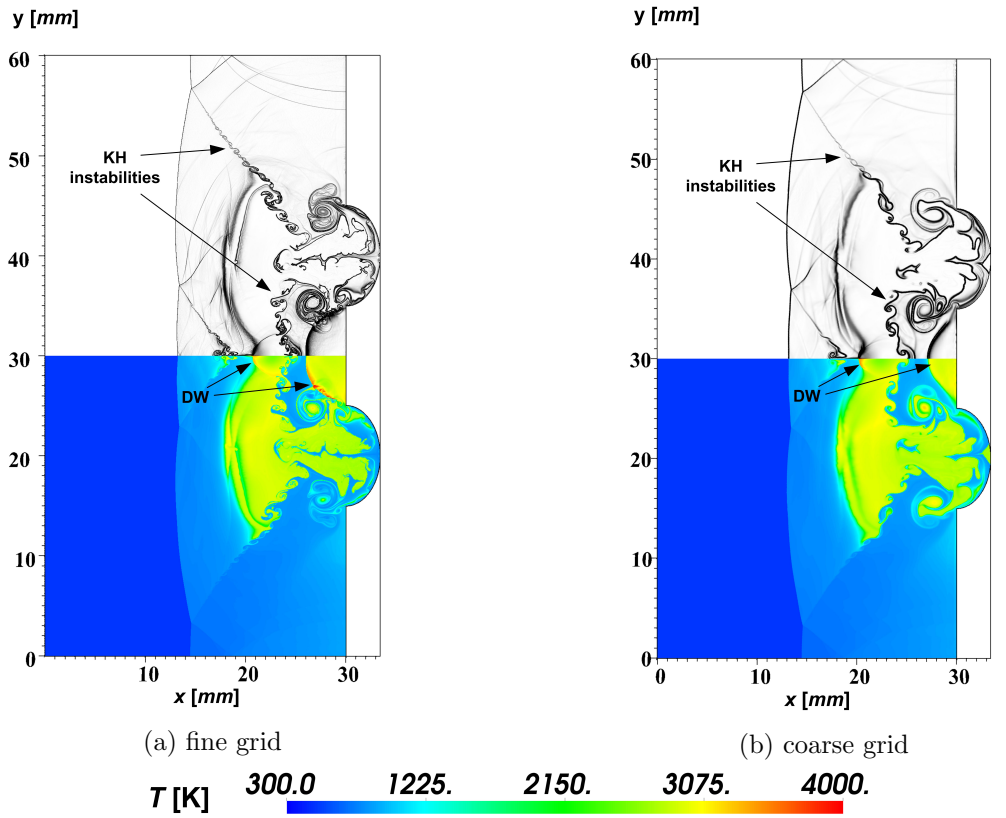



**Figure 3.** Parallel speedup on supercomputer MVS-10P

Let us consider the process of detonation wave initiation in the case of a numerical grid consisting of approximately 28 million triangular cells. The reflection of the incident plane SW from the end of the wall is associated with the formation of a series of waves that interact with each other and with the walls of the channel. The presence of vertical walls leads to an

amplification in the gasdynamic parameters inside the elliptic cavities. Ignition of the mixture occurs in the region of focusing of the flow at about 20 $\mu s$. During the combustion of the mixture, the formation of combustion waves propagating from the ignition region occurs. Detonation initiation occurs at about 41 $\mu s$ in two regions on the symmetry axis of the channel outside the elliptic cavities. Figure 4a shows the spatial distribution of temperature (lower half of the picture) and density gradients (upper half of the picture) at 41 $\mu s$. An important role in the considered process of detonation initiation is played by the interference of combustion zones and waves formed after the reflections of the incident SW from the profiled end wall. The presence of regions with distributed elliptic surfaces leads to a decrease in the detonation initiation time compared to the case when the rectangular channel without a profiled end is considered. This statement is in agreement with both experimental [1] and numerical [5] works.

A series of calculations of detonation initiation in the channel with the proposed geometry is carried out. Numerical grids with different numbers of triangular cells are considered: 1.2 mln, 6 mln, 18 mln and 28 mln cells. The spatial distribution of temperature and density gradients on the grid consisting of 1.2 mln cells at 41 $\mu s$ are shown in Fig. 4b. The results obtained using different grids correspond to each other. In particular, the initiation of the mixture in all calculations occurs at about 41 $\mu s$. However, the detailed resolution of elements and structures such as the Kelvin–Helmholtz instability formed during the gas flow is observed on the most detailed grids. On the detailed grids the thickness of SWs becomes smaller that is associated with a decrease in the effect of numerical smearing in calculations.




(a) fine grid

(b) coarse grid

**Figure 4.** Predicted numerical schlieren images (upper half) and temperature distributions (lower half) at the time instant 41 $\mu s$

## Conclusions

A parallel computational algorithm for calculating gasdynamic flows with detonation waves on unstructured triangular grids is proposed. Parallelization of the computational algorithm is conducted by the domain decomposition method using the METIS library. Data exchange between computing cores is carried out using MPI library functions. The acceleration of the realized computational algorithm in the problem of detonation initiation in a model hydrogen-oxygen mixture is demonstrated. Calculations of detonation initiation on several numerical grids with different numbers of triangular cells are carried out. The results show that the detonation initiation patterns obtained using different grids correspond to each other. Detailed resolution of flow structures, including Kelvin–Helmholtz instabilities, is observed on computational grids with a large number of triangular cells.

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