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Second-order Godunov-type scheme for reactive flow calculations on moving meshes

Boris N. Azarenok [a,*], Tao Tang [b]

[a] Dorodnicyn Computing Center of the Russian Academy of Sciences, Vavilov Street 40, GSP-1, Moscow, 119991, Russian Federation
[b] Department of Mathematics, The Hong Kong Baptist University, Kowloon Tong, Hong Kong

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Abstract

The method of calculating the system of gas dynamics equations coupled with the chemical reaction equation is considered. The flow parameters are updated in whole without splitting the system into a hydrodynamical part and an ODE part. The numerical algorithm is based on the Godunov's scheme on deforming meshes with some modification to increase the scheme-order in time and space. The variational approach is applied to generate the moving adaptive mesh. At every time step the functional of smoothness, written on the graph of the control function, is minimized. The grid-lines are condensed in the vicinity of the main solution singularities, e.g., precursor shock, fire zones, intensive transverse shocks, and slip lines, which allows resolving a fine structure of the reaction domain. The numerical examples relating to the Chapman–Jouguet detonation and unstable overdriven detonation are considered in both one and two space dimensions.

Keywords: Detonation wave; Second-order Godunov-type scheme; Moving mesh

1. Introduction

Modeling detonation wave motion in gases has started in 1940s, see, e.g. [26,59], based on the theory of the steady one-dimensional detonation, referred to as the Zeldovich–Neuman–Doering (ZND) model. The early computations were rather rough giving only a qualitative estimate to the solution. The main difficulty of the numerical simulation is due to the different scales of the flow domain and chemical reaction zone.

* Corresponding author. Tel.: +7 95 135 6498; fax: +7 95 135 6159.
E-mail addresses: azarenok@ccas.ru (B.N. Azarenok), ttang@math.hkbu.edu.hk (T. Tang).

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Thus, the simulation for the real objects requires using more powerful computers or more sophisticated numerical algorithms.

Developing the numerical algorithms is executed in several ways. In the first group the burning zone is not resolved by the grid points. Instead in [16] the chemical heat release is put into the Riemann problem. This idea is used in [28] as well. In [15], the chemical reaction term is present only to the energy equation, the kinetics equation is omitted and the Riemann problem is formulated for the non-reactive gas. Although the detonation wave speed is obtained rather inaccurately, the calculations of the real industrial objects with complex geometry are found satisfactory. In the second group of the algorithms, the burning zone is resolved by putting there several grid points in the normal direction. This requires to use very fine quasiuniform meshes. In the most of these algorithms one applies the fractional step approach (also referred to as the Strang splitting schemes). At each time step, first, the system of conservation laws is treated and then the ODE to the kinetics equation is solved, e.g., see [8,17,30,44,45,54]. Although the convergence of the fractional step method was justified theoretically for scalar conservation laws with source terms [19,52,53], the application for this approach for hyperbolic system with stiff source terms generally produces the non-physical solution, e.g., see [17]. Another way is to treat the system of conservation laws coupled with the reactive equation as a whole, i.e., using the unsplit schemes. In this approach the heat release term in the right part of the system is treated as a source term. In [7], the generalized Riemann problem is introduced for the reactive equations to provide the second-order approximation in time. In [20], the detonation process is simulated on the Lagrangian mesh. Space-time paths are introduced in [43] on which the equations are reduced to the canonical form about the "new" Riemann invariants. All the above methods are of Godunov-type (except [16], where the random choice method is used), i.e., include solution of the Riemann problem that allows obtaining the narrow wave front rather precisely. In contrast to it, the random projection method is used in [6] where the Riemann problem is omitted from the consideration. However, justification of such a simplification is still under the question. Some other non-Godunov-type algorithms can be found in [42].

In this work, we present an unsplit scheme for calculating the reactive flow equations on the moving meshes. For this we utilize the idea of the Godunov's scheme on the deforming meshes (see the monographs [1,32]), when the conservation laws are written in the integral form using the so-called generalized formulation in $\mathbb{R}^3$ space (x, y, t) (t is time). This allows updating the flow parameters directly on the moving curvilinear mesh without using interpolation. One implementation of the first-order Godunov's method on the moving mesh with front tracking was performed in [27]. In some sense such a kind of schemes can be referred to as an ALE approach, cf. [29].

In [2], a modification of the Godunov's scheme of the second-order accuracy in time and space was suggested, because the first-order original scheme in [32] does not provide proper grid-nodes adaptation to the solution singularities. The second order in space is achieved by interpolating the flow parameters inside the cells, and in time by using the Runge–Kutta method with a predictor–corrector procedure. To obtain the fluxes value at the cell sides the Riemann problem is solved. The kinetics equation is treated similarly, namely we write it in the integral form and approximate it in the hexahedron cell in space (x, y, t).

The variational approach is employed to generate the moving mesh. The variational approach to generate two-dimensional meshes was suggested in the form of quasi-conformal mapping in [31]. In [56], the variational principles for constructing the adaptive moving grids in the gas dynamics problems were formulated. They introduced the measure (or functional) of mesh deviation from the Lagrange coordinates, measure of mesh deformation and mesh concentration. In [10], the functional of smoothness was applied, to which the Euler–Lagrange equations coincide with the system used in [58]. In [40], the problem of minimizing the functional of smoothness (also referred to as the harmonic or Dirichlet's functional) written for a surface of the control/monitor function was formulated to construct an adaptive-harmonic mesh. Other forms of the monitor functions for the harmonic functional have been considered in [11,21,51]. In continuous approach the harmonic mapping, subject to some known conditions, is a homeomorphism. However, its discrete realization, based on solving the Euler–Lagrange equations, suffers from mesh tangling in the