



Accumulation of errors in numerical simulations of chemically reacting gas dynamics



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ABSTRACT

The aim of the present study is to investigate problems of numerical simulations precision and stochastic errors accumulation in solving problems of detonation or deflagration combustion of gas mixtures in rocket engines. Computational models for parallel computing on supercomputers incorporating CPU and GPU units were tested and verified. Investigation of the influence of computational grid size on simulation precision and computational speed was performed. Investigation of accumulation of errors for simulations implying different strategies of computation were performed.

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1. Introduction

Detonation combustion mode has definite exceptional properties as compared with classical deflagration mode used in modern engines. Those differences are: extraordinary higher rates of flame propagation (four orders of magnitude higher), higher pressure and temperature values in reaction zone, minimal entropy production for Chapman–Jouguet regime. Unsteady-state transition processes between two combustion modes are possible. Uncontrolled detonation onset in engines could be an explosion hazard. That is one reason numerical simulations and predictive modeling of detonation onset are necessary for providing safety regulations. On the other hand control of detonation onset is necessary in perspective pulse detonation engines, which are under development now [1–7]. In our numerical studies we'll take hydrogen fuel as an example. The advantages of a constant

volume combustion cycle as compared with constant pressure combustion in terms of thermodynamic efficiency has focused the search for advanced propulsion on detonation engines [8,9]. Numerical simulations of pulse detonation engines operation aimed at increasing their efficiency and developing control strategies consume much time and computational resources. Parallel computing technologies and developing effective schemes aims at reducing the simulation time. The thermodynamic efficiency of Chapman–Jouguet detonation as compared with slow combustion modes is due to the minimal entropy of the exhaust jet [1]. Extensive numerical multidimensional simulations of detonation onset and propagation are necessary in combustion chambers able to distinguish optimal scheme for the operation cycle. Parallel computing is a powerful tool enabling to make simulations more effective and less time consuming. However solving numerical problems it is necessary to control accumulation of numerical error. For fine grid simulations of unsteady-state processes numerical time step is being chosen based on Courant criterion, which makes it also small. Thus the number of time steps could be enormous.

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Keeping in mind that each time step contributes to accumulation of numerical error, the number of time steps should be limited so as the accumulated error did not exceed 100%.

The aim of the present study is developing mathematical model for evaluation of stochastic numerical errors accumulation in multistep simulations of chemically reacting gas dynamic processes in rocket and detonation engines. Effectiveness of different numerical schemes and its parallelization potential for supercomputing will be also investigated. The role of supercomputer architecture will be discussed.

2. Mathematical model

2.1. Equations

In order to calculate multicomponent gas dynamics with chemical reactions excluding transport phenomena effects and considering external mass and energy sources we use the following set of simultaneous equations:

$$\frac{\partial \rho_k}{\partial t} + \frac{\partial}{\partial x_j}(\rho_k u_j) = \dot{\omega}_k + \dot{M}_k; \tag{1}$$

$$\frac{\partial \rho u_k}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j) + \frac{\partial p}{\partial x_i} = 0; \tag{2}$$

$$\frac{\partial}{\partial t} \left(E + \rho \frac{\mathbf{u}^2}{2} \right) + \frac{\partial}{\partial x_j} \left(\left(E + p + \rho \frac{\mathbf{u}^2}{2} \right) u_j \right) = \dot{Q} + \dot{Q}_m. \tag{3}$$

In Eqs. (1)–(3) index k takes values 1 ... N_c (number of components) and indices i, j – values 1, 2, 3 (number of dimensions); repeated indices presume summation. In total there are $N_c + 4$ differential equations in the set.

2.2. Algebraic relations

Differential Eqs. (1)–(3) are to be complemented with three algebraic relations and algebraic representations for chemical and mass and energy sources. First three relations will look like:

$$\rho = \sum_{k=1}^{N_c} \rho_k, \quad p = R_G T \sum_{k=1}^{N_c} \frac{\rho_k}{W_k},$$

$$E = R_G T \sum_{k=1}^{N_c} \frac{\rho_k}{W_k} \left(\hat{H}_k(T) - 1 \right). \tag{4}$$

Relations (4) define gas density ρ , pressure p and internal energy per unit volume E of mixture respectively. Other definitions are: R_G is universal gas constant, W_k is molar weight of a component, and for temperature functions – $\hat{H}_k(T)$ is dimensionless enthalpy of a component encompassing enthalpy of formation at given temperature T_{ref} (“chemical energy”). More precisely the conception of dimensionless thermodynamic data is given in Ref. [1]. As these expressions show, in algebraic expressions here and in what follows it is often convenient to use molar density X_k

(which sometimes, especially in chemical literature, is called “concentration”) instead of partial component density ρ_k :

$$X_k = \frac{\rho_k}{W_k}. \tag{5}$$

Mass source $\dot{\omega}_k$ is due to chemical interactions present in the system of gases. Mass source \dot{M}_k results from the external source outcome. Source \dot{Q}_k in energy equation is a total income of energy carried with the external mass \dot{M}_k ; source \dot{Q} in energy equation denotes extra energy income from the external source. Thermal energy source implying chemical reactions inside the system is absent in this model because energy E already encompasses chemical energy of each component. External sources are not directly linked chemical interactions inside the system; they aim to inject mass and energy in gas mixture from the outside for ignition and movement excitation. In our problem setup they explicitly depend on time and location.

Chemical sources $\dot{\omega}_k$ for most systems take a complicated form; they can be expressed depending on temperature T and set of the molar densities $\mathbf{X} = \{X_k\}$; sum of these sources equals zero due to the law of mass conservation in chemical reactions:

$$\dot{\omega}_k = W_k \hat{\omega}_k(T, \mathbf{X}), \quad \sum_{k=1}^{N_c} \dot{\omega}_k = 0. \tag{6}$$

There also exist more precise laws of chemical interactions (law of mass conservation for each element), which are taken into account in kinetic mechanism and can be considered in numerical realization of the model for calculation simplification and precision improvement. General form of chemical sources is quite complicated and includes members which are nonlinear for each argument; the common view is

$$\omega_r = M_r(\mathbf{X}) \left[k_{F,r}(M_r, T) \prod_j X_j^{\alpha_{r,j}} - k_{B,r}(M_r, T) \prod_j X_j^{\beta_{r,j}} \right], \tag{7}$$

where ω_r is speed (intensity) of reaction r , $\nu_{r,k}$ is an algebraic stoichiometric coefficient of a component k in reaction r , M_r is a third bodies influence coefficient (those which do not change) in the reaction r , which equals 1 when this influence is absent, $k_{F,r}$ is a speed coefficient of a forward reaction, usually depending solely on temperature, but for some (“out-of-order”) reactions also of M_r , $k_{B,r}$ is a speed coefficient of the backward reaction, $\alpha_{r,j}$ are powers of components in the forward reaction (usually, but not always nonzero only for incoming components) $\beta_{r,j}$ are powers of components in the backward reaction.

Dependencies $\hat{H}_k(T)$ are often expressed as polynomials with different coefficients for different components [10].

In practice Eq. (1) can be used transformed to the following view:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = \dot{M} = \sum_k \dot{M}_k; \tag{8}$$

$$\frac{\partial Y_k}{\partial t} + u_j \frac{\partial Y_k}{\partial x_j} = \frac{\dot{\omega}_k + \dot{M}_k}{\rho} = S_k. \tag{9}$$

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