Eulerian Numerical Techniques EGAK and TREK for Simulation of Multidimensional Multimaterial Flows

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The paper presents overview of main algorithms underlying Lagrangian-Eulerian techniques EGAK and TREK for simulation of 2D and 3D multimaterial flows with large deformations, including the turbulent mixing phase. Some results of computations are presented that give an estimate of the technique accuracy and efficiency.

Introduction

Use of Eulerian and arbitrary Lagrangian-Eulerian (ALE) techniques for shock-wave multi-material continuum flows becomes more and more significant owing to their advantages, as compared to Lagrangian techniques, and of most importance among these advantages are that they provide crash-proof computations, easier preparation of initial data, less labor-intensity and less dependence of results on the computation executor skills.

However, despite of their attractiveness Eulerian techniques require resolving a number of complex problems. The main of these problems are the following:

1. Lagrangian gas dynamics equation approximation for a multi-material medium because of occurrence of the so-called mixed cells containing two and even more materials.
2. A lower accuracy, as compared to Lagrangian methods, due to the need in solving the advection equation and scheme viscosity occurred as a result of it.
3. Determination of interface positions and computation of their motion over the immovable computational grid.
4. Problems of simulation of various physical processes, namely: HE burning and detonation, heat transfer, elasticity-plasticity, etc.
5. Necessity of using of a heterogeneous grid.
6. The problem of efficient parallelization during implementation of codes on parallel computers.

The efficiency and accuracy of Eulerian techniques depend on resolution of the problems above. The algorithms used to improve the efficiency and accuracy of techniques EGAK (2D) and TREK (3D) are described below.

Note that although EGAK and TREK techniques are mainly used for computations on immovable grids, ALE approach is used in them for implementation of codes. Thus, equations are approximated in two phases: Lagrangian and Eulerian. A single computational grid is used that can

move rather arbitrarily during computations. The computational grid cells are quadrangles in 2D case and hexahedrons, if it is 3D case. Components may be different: various materials with their own equations of state (EOS); various phase states of any of the materials, such as HE-EP, water-vapor, etc.; various fractions of a dispersed impurity; vacuum; and ideal solids.

It's impossible to describe all algorithms of codes within one paper. So, in the description below the problems solutions to which are specific for the techniques under consideration are in focus of our attention.

Lagrangian Gas Dynamics Methods for Calculation of Mixed Cells

Principal equations and assumptions

It is assumed that a computational region may have several components (materials) having different EOS. The material interfaces may be not coincident with the computational grid lines, moreover, availability of mixtures in the computational domain with no interfaces between them is possible. Mixtures are heterogeneous, in general, and each material can have its own EOS, however, homogeneous mixtures are also possible. A single-velocity model of the multi-material medium is used, with each material of this medium being described by a complete set of thermodynamic parameters: density, specific internal energy, and volume concentration.

Velocity $\vec{u}$ is defined at the computational grid nodes, scalar quantities ρ_i, e_i, P_i, P, $\beta_i=V_i/V$ are defined at the centers of cells; here ρ is density; **e** is specific internal energy; **P** is pressure; **V** is volume; β is volume concentration; **i=1,…,J** is the number of material.

The original system of differential equations of multi-material gas dynamics has the form:

$$\frac{d\vec{u}}{dt} = -\frac{1}{\rho}\,\mathrm{grad}(P+q) \qquad [1]$$

$$\frac{d\rho_i}{dt} = -\rho_i \mathrm{div}\vec{u}_i \qquad [2]$$

$$\frac{d\beta_i}{dt} = \beta_i\left(\mathrm{div}\vec{u}_i - \mathrm{div}\vec{u}\right) \qquad [3]$$

$$\frac{de_i}{dt} = -\frac{P_i + q_i}{\rho_i}\mathrm{div}\vec{u}_i \qquad [4]$$

Here q and q_i are computational viscosities; $i=1,2,\ldots,J$.

The system of Eqs.1-5 is closed by EOSes of materials.

$$P_i = P_i\left(\rho_i, e_i\right) \qquad [5]$$

Equation 3 is a consequence of Eq.2, it is given here to emphasize that in case of a multi-material medium the volume concentrations should be also found at a new time point.

The paper considers only the problems related to calculation of mixed cells. For this reason, the difference equations below are given only in the necessarily required number, for example, with omitted details of differential operator approximation in space.

The system of Eqs.1-5 is open, in particular, pressure **P** for the medium, as a whole; material divergences $\mathrm{div}\vec{u}_i$; artificial viscosity **q** of a cell, and artificial viscosities of its materials $\mathbf{q_i}$ are not determined. To close the system of equations, additional assumptions concerning the state of mixtures in mixed cells are required.

Main closure methods

Till recent time, an assumption of equal compressibility of materials (Bakhrakh et al., 1984) was the only assumption used in practice

$$\mathrm{div}\vec{u}_i = \mathrm{div}\vec{u} \qquad [6]$$

Let the method based on this assumption be **method 1.**

We also use **method 2** based on assumption of equal pressures of materials (components) with regard to their viscosities of the form

$$P_i + q_i = P_k + q_k \qquad [7]$$

Such assumption leads to the iteration algorithm of solving the system of Eqs.2, 4, and 5 (Zharova and Yanilkin, 1992).

Method 3 is also used**,** it has been proposed in the paper by Bondarenko and Yanilkin, 2000 and is based on the assumption of equal material pressure increments. The method leads to the iteration-less algorithm that shows a significantly higher accuracy of computations for problems with mixtures, as compared to the method 1. The method 3 is based on closing relations $\Delta P_i = \Delta P_k$, or

$$\rho_i c_i^2 \mathrm{div}\vec{u}_i = \rho_k c_k^2 \mathrm{div}\vec{u}_k \qquad [8]$$

With regard to $\sum \beta_i \mathrm{div}\vec{u}_i = \mathrm{div}\vec{u}$ (that follows from the requirement of additivity of material volumes) we obtain the following system of equations to find $\mathrm{div}\vec{u}_i$. Solution of this equation system gives

$$\mathrm{div}\vec{u}_i^n = \mathrm{div}\vec{u} \frac{1}{\sum_k \frac{\beta_k^n}{\rho_k^n \left(c_k^n\right)^2}} \cdot \frac{1}{\rho_i^n \left(c_i^n\right)^2} = \xi_i \mathrm{div}\vec{u} \qquad [9]$$

In the paper by Goncharov and Yanilkin, 2004 the method 3 was modified by introduction of the material pressure equalization algorithm (**method 3P**) that significantly increased the method accuracy.

The following problem gives notion of the comparative accuracy of the methods above.

Problem 1. A shock wave propagation through a mixture of two gases

The following problem is of interest. There is a mixture of two gases within the region 0<x<100, the gases are in completely mixed and equilibrium state (P=0, u=0). The first gas has density ρ=1 and adiabatic exponent γ=3, the second gas parameters are ρ=1 and γ=1.2. Constant velocity u=2 is specified on the left boundary. A shock wave is propagating through the gas mixture, maximum levels of compression separately for each gas (i.e. ρ=2 for the first gas and ρ=11 for the second one) have to be achieved on this shock wave provided that there is no adiabatic exchange of energy between the two gases. The material pressures must be equal. The computational domain is uniformly partitioned into 100 cells. The computations are carried out in Lagrangian statement.

Results of the computations carried out are given in Fig.1 for the three methods above in the form of pressures (mean pressure and pressures of materials) depending on the distance at time t=25. Fig.5 gives the similar profiles of material densities.

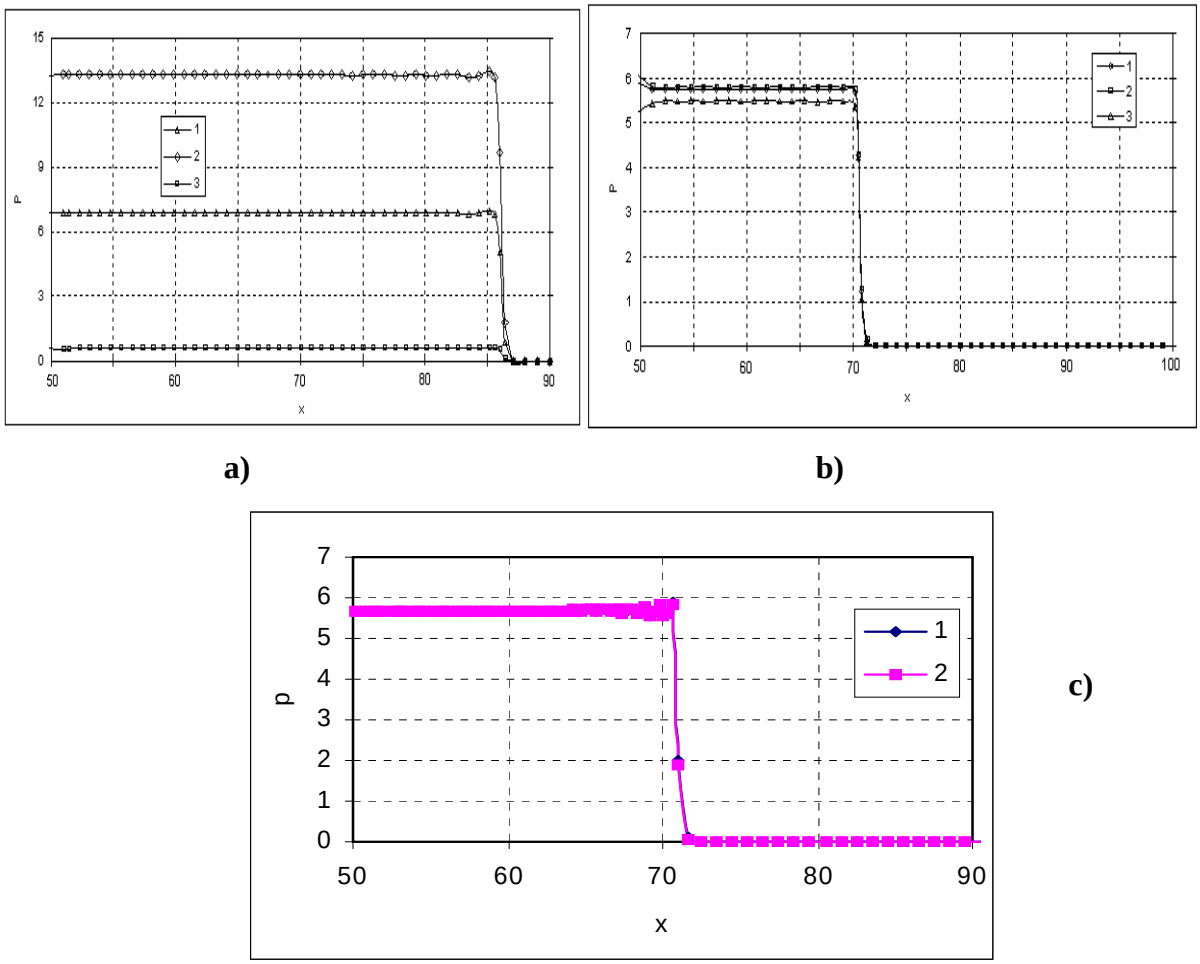
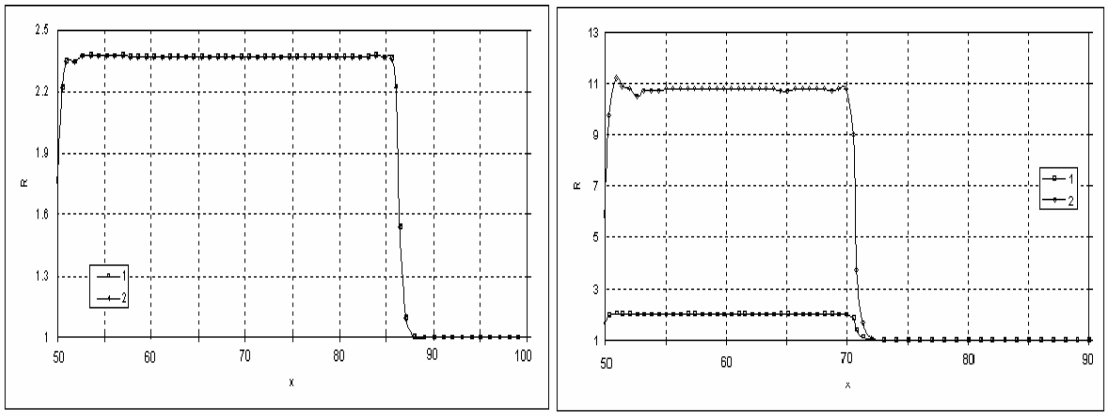
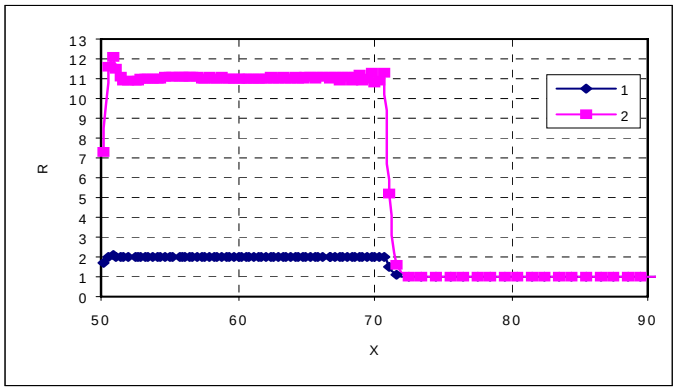


Figure 1. Pressure profiles in problem 1, t=25: a)-method 1, b) - method 3, c) - method 3P; 1 – mean pressure; 2 – pressure of material 1; 3 – pressure of material 2.



a) **b)**



c)

Figure 2. Density profiles in problem 1, t=25: a)-method 1, b) -method 3, c) - method 3P; 1 – density of material 1; 2 – density of material 2.

When analyzing the computation results, we want to point out that in computations with method 3 the mean pressure profiles differ from each other, however, they are close enough and the shock wave propagation velocities are also close. Computation with method 1 gives noticeably different results, both in the amplitude of pressure behind the shock wave front and in the front motion velocity. In this computation material pressures strongly differ from each other and the mean value, while in computation with method 3 they are close, though not completely coincident, as it takes place in computations with material pressure equalization. Computation using method 3P almost completely coincides with computation using method 2 (Bondarenko and Yanilkin, 2000) that uses the assumption of equal material pressures.

The density profiles also show that method 1 gives a result which accuracy is unacceptable. The both material densities are equal in this computation in full accordance with the assumption adopted, with the only exception that the first material undergoes overcompression and the second one - undercompression. Methods 2 and 3P are more accurate than method 1. The compression values obtained using these methods behind the shock wave front are close to the expected ones. At the same time, it is clear that method 3P is the most preferable one among the three methods under consideration (because densities behind the wave front virtually coincide with the expected values).

Thus, the calculated data shows that method 3P is somewhat better in accuracy than method 3 and have certain advantages, as compared to method 1.

Approximation to the Advection Equation

Specific features of using CM, DM, and PPM methods

One of the most successful among the methods in use that allow improving the solution accuracy of the advection equation for a multi-material case is the method of concentrations (CM) proposed in the paper by Bakhrakh et al., 1981. This is the method underlying EGAK and TREK techniques and its first version was developed exactly for EGAK.

In the CM method, their own individual parameters of thermodynamic states (the number of these parameters increased, as the method developed) are used for various materials. For gas dynamics, a complete set of parameters includes densities (or mass concentrations (fractions), the method is called after them) energies and volume concentrations (fractions). The continuity equations and energy equations are written for each material separately. The idea of CM method is that a special algorithm based on local reconstruction of interface positions over the field of concentrations is used to calculate flows moving out of mixed cells. The method allows localization of the interface positions up to one computational cell. We'll not describe all algorithms of the method, they have been already described in details in various papers, for example, see the review paper by Yanilkin, 1999. Here we consider only some problems rising, if the method is used in combination with DM and PPM.

The equation for material volume flows across a cell side (face) can be written, in general, as

$$\Delta V_i = \Delta V \cdot \beta^i_{\Delta V} \qquad [10]$$

Here, ΔV is the total volume flow across the current face, $\beta^{\mathrm{i}}_{\Delta \mathrm{V}}$ is some volume concentration value for the i-th component. For $\beta^{\mathrm{i}}_{\Delta \mathrm{V}}$ calculation the following 3 methods are possible depending on situation: method DM, method CM and method PPM. If it has been managed to reconstruct the interface position in a donor cell basing on the field of concentrations, CM is used, otherwise use PPM method. PPM method is actually used for calculation of flows going out of one mixed cell to another mixed cell or out of a mixed cell to a pure cell (if there is a thin layer of another material in this cell).

After the material volume flows has been found, the mass flows are to be found using a similar equation

$$\Delta \mathrm{M}_{\mathrm{i}} = \Delta \mathrm{V}_{\mathrm{i}} \cdot \rho^*_{\mathrm{i}} \qquad [11]$$

where ρ^*_{i} is the value of density in flow to be determined either by the donor method or PPM method. If the volume flow has been calculated using CM method, density is calculated using DM method, otherwise PPM method is used.

To calculate fluxes of energy and other quantities determined per unit mass of material, use the same approach, however, in Eq.11 $\Delta \mathrm{M}_{\mathrm{i}}$ is used instead of $\Delta \mathrm{V}_{\mathrm{i}}$ and the corresponding value instead of ρ^*_{i}.

The procedure of using various methods in EGAK and TREK techniques is described in more details in papers by Kucherova and Yanilkin, 2003 and Yanilkin, 2004. Here we only describe some specific features of using PPM in TREK technique due to parallelization. The matter is that in order to calculate a flow across any cell side this method requires data on the state in 5 cells; in TREK

code only data from one layer of near-boundary cells is transmitted from one processor to another. In view of this fact, situations are possible, when a standard PPM method cannot be used in it original form and, hence, some modifications to the algorithm are required.

Case 1. Look at Fig.3, where cells 1, 2, and 3 are in processor 1, while cells 4 and 5 are in processor 2. It is required to calculate (using PPM method) the flow moving from the right to the left across the common edge of cells 2 and 3 in processor 1. In such a case PPM method requires all the cells shown in Fig.3.

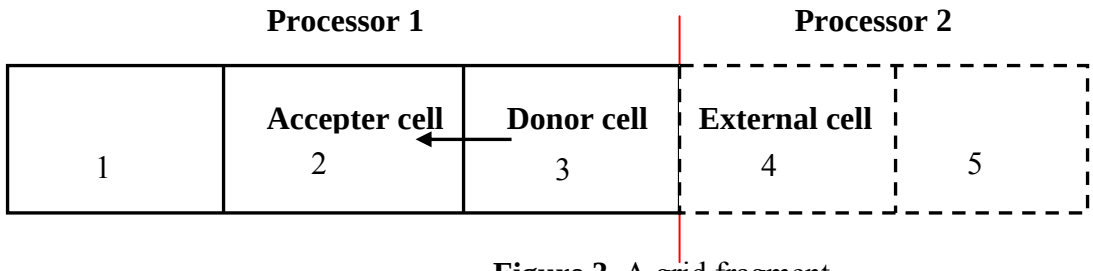


Figure 3. A grid fragment

As one can see from Fig.3, only 3 of 5 required cells are in processor 1. Besides, we know the state of cell 4 from processor 2, however, we don't know the state of cell 5. To use standard algorithms of PPM method, the state of cell 5 is copied from the near-boundary cell (from cell 4, in our case). So, we now have all the data needed for PPM method operation.

Case 2 is shown in Fig.4. It is required to calculate a flow across the common edge of cells 3 and 4 using PPM method. In this case the flow can be calculated both on processor 1 and processor 2. Thus, one and the same flow across the common face of cells 3 and 4 can be calculated in different manners (see case 1) depending on what processor is the flow calculated. For this reason DM method is always used to avoid ambiguity.

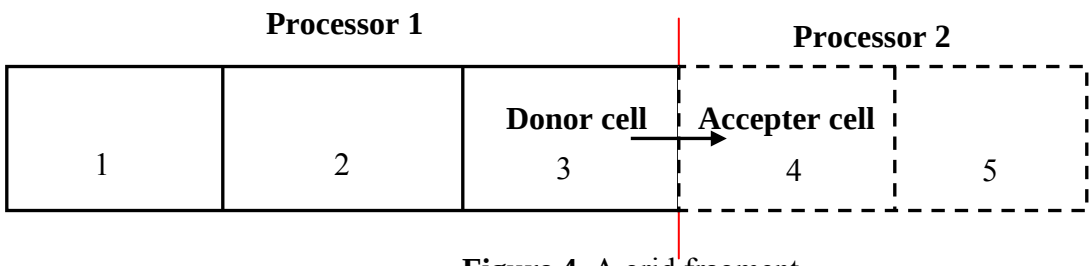


Figure 4. A grid fragment

As computations show, these and some other exceptions insignificantly affects the results of multiprocessor computations. Further we give two examples of using the methods described above.

Problem 2. Explosion in exponential atmosphere.

At initial time, a material of density ρ=1 and internal energy $e = \frac{E}{4/3\ \pi R_0^3 \rho}$ $(E = 1)$ is contained in exponential atmosphere $\rho = \rho_0 \exp(-x)$, $\rho_0 = 1$, inside a region of radius R=0.75 and the center at point x=0. It is known that at time t~35 the so-called breakthrough of a shock wave takes place, when its velocity tends to infinity. Results of this problem computation using DM and PPM methods in 2D approximation are shown in Fig.5 in the form of internal energy of atmosphere and in Fig.6 in the form of X-t diagram of the shock wave front moving upwards. One can see from

a)

Fig.6 that DM method gives a qualitatively incorrect result, which doesn't become better, as the size of cells decreases. PPM method allows obtaining a result to an acceptable accuracy.

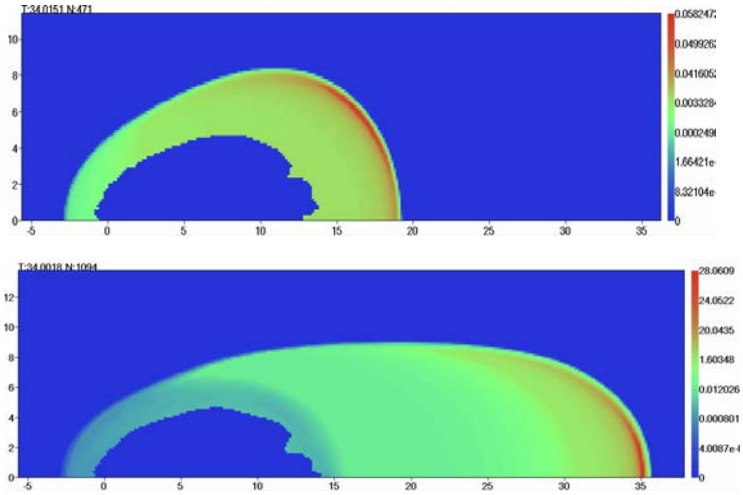


Figure 5. The internal energy of the atmosphere, t=34, a) method DM, b) method PPM.

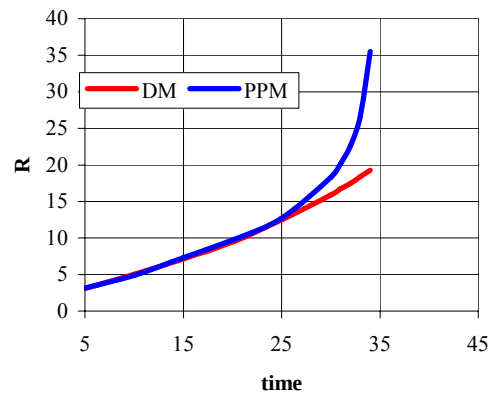


Figure 6. The dependence of the shock wave radius on time.

Approximation to the Heat-Transfer Equation

With approximation to the heat-transfer equation in mixed cells, it is required to introduce additional (as compared to gas dynamics) closure relations. Currently, the assumption of instant equalization of material temperatures in mixed cells is widely used for heat transfer computations. Besides, the method based on the assumption of heat exchange between mixed cells' materials is also used in EGAK and TREK techniques.

The main idea of the method consists in dividing the heat transfer process into two phases. During the first phase a common heat transfer equation for mean energy of a medium is solved and during the second phase heat exchange between materials inside mixed cells takes place.

Solution of the heat-transfer equation for mean energy (phase 1)

Consider the heat-transfer equation

$$\rho \frac{\partial e}{\partial t} = \mathrm{div}(\chi \cdot \mathrm{grad}T) \qquad [12]$$

where ρ, e, χ, T are averaged parameters of medium: density, specific internal energy, coefficient of heat conductivity, and temperature.

The grid functions of density, specific internal energy and temperature are specified at the center of cell and heat flows are specified on the cell's sides (faces). Equation 12 is approximated using the implicit difference scheme

$$\frac{e^{n+1} - e^{n}}{\tau} = \left(\frac{\mathrm{div}\left(\chi \cdot \mathrm{grad}T\right)}{\rho} \right)^{n+1} \qquad [13]$$

To solve the system of finite-difference Equations 13, any difference scheme can be used. The solution technique for a 2D case is described in the paper by Bondarenko et al., 2000. In 3D case

the method of local iterations proposed by Lokutsiyevsky and Lokutsiyevsky, 1984 and modified by Zhukov, 1986 is used. The method is based on the use of the operator of layer-by-layer transition, which is a cycle of **s** elementary steps, with each of the steps being equivalent in labor-intensiveness to one step of the traditional explicit scheme. The method is appropriate for implementation on parallel machines.

Computation of heat exchange between materials (phase 2)

Upon the completed phase 1, mean flows of heat across the cell faces are known. During the second phase these flows in mixed cells are distributed over materials, then heat exchange between the materials across the inter-material interface is performed. For a case of two materials in one cell, the process is described using the following system of difference equations:

$$\begin{cases} M_1 \dfrac{e_1^{n+1} - e_1^n}{\tau} = S_{12}\chi_{12} \dfrac{T_2^{n+1} - T_1^{n+1}}{L_{12}} + \sum_{j=1}^{6} Q_{1,j} \\ M_2 \dfrac{e_2^{n+1} - e_2^n}{\tau} = -S_{12}\chi_{12} \dfrac{T_2^{n+1} - T_1^{n+1}}{L_{12}} + \sum_{j=1}^{6} Q_{2,j} \end{cases} \qquad [14]$$

Here, M_i are masses of materials; e_i are specific internal energies of materials; χ_{12} is the mean coefficient of heat conductivity for inter-material heat exchange. S_{12} is the area of contact between the materials (i.e. the, cross-section area); L_{12} is the distance between the centers of volumes occupied by materials; $Q_{i,j}$ is the heat flow of the i-th material across the j-th face.

To illustrate the foresaid, Fig.7 shows a mixed cell in 2D cross-section with the drawn interface and the quantities from Eq.14.

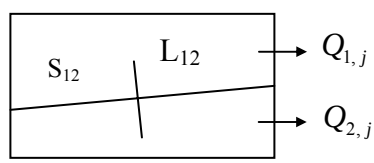


Figure 7. A 2D cross-section of a mixed cell.

In our techniques, positions of interfaces in mixed cells are reconstructed basing on the field of concentrations. The algorithms of determining interfaces and quantities mentioned above are described in the paper by Bondarenko et al., 2000. Note that in 2D case an interface is approximated with a straight-line segment and in 3D case – with a plane. Distribution of heat flows across faces of cells between components is calculated using the equation

$$Q_i = Sq \frac{S_i \chi_i}{\sum_{k=1}^{2} S_k \chi_k}, \quad i = 1, 2 \qquad [15]$$

i.e. in proportion to heat conductivity coefficients and areas. In Eq.15 **q** is the mean flow of heat (calculated during phase 1) per unit area entering a cell across its face; S is the face area; S_i is a portion of the face area occupied by the i-th material; χ_i is the heat conductivity coefficient of the i-th component related to the face.

Equations 14 is solved by iterations using Newton method. The solution process results in new values of temperatures and internal energies of materials.

Problem 3. Heat exchange in a two-component medium

A plane divides a rectangular parallelepiped into two parts. The first region contains a hot light gas (ρ_1=0.1, e_1=10, χ_1=1, c_V=1) and the second one contains a cold heavy gas (ρ_2=10, e_2=1, χ_2=0.5, c_V=1). Zero flows are specified on boundaries. The settings of computations carried out were the following: the material interface coincides with the computational grid lines (**Lagrangian** computation); the material interface doesn't coincide with the computational grid lines, with an assumption of equal temperatures of materials in mixed cells (**method 1**); the material interface doesn't coincide with the computational grid lines, heat exchange between materials takes place (**method 2**). The problem is one-dimensional, however, computations were carried out in 3D geometry.

The computation results are shown in Fig.8.

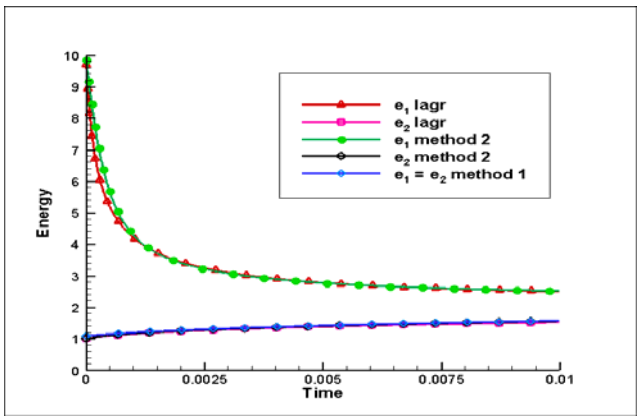
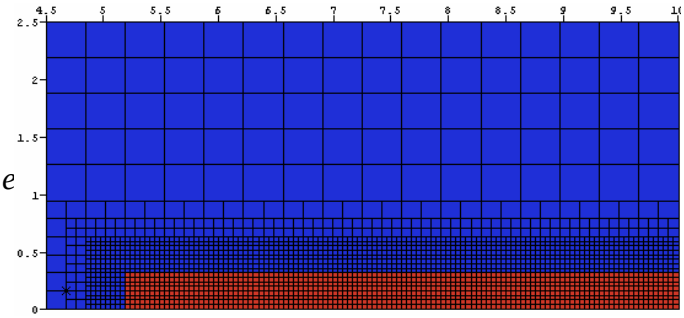


Figure 8. The curves of specific internal energy of materials versus time for materials inside a mixed cell, the energies for two neighboring cells are given in case of Lagrangian computation.

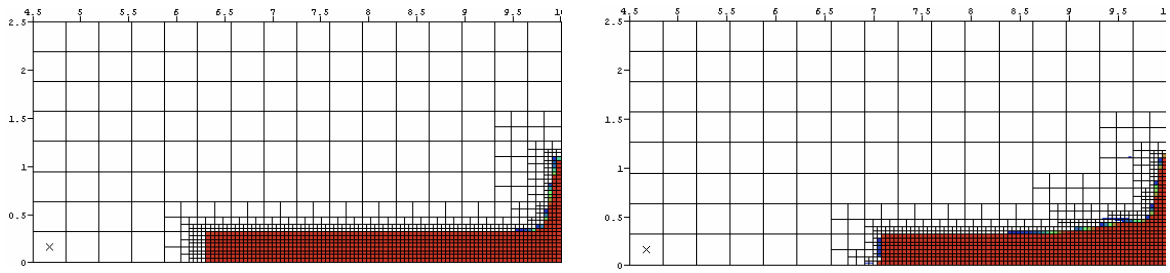
Use of an Adaptively Built-in Refined Grid

For the sake of 2D computation accuracy improvement and run-time reduction, EGAK technique uses an adaptively built-in refined computational grid (this procedure is not implemented for 3D case). The main features of such a grid are as follows: new cells are built of segments passing across mid points of sides of larger cells; the method of refining cells is the same at all levels; the maximum number of refinement levels is 5; the difference between neighboring cells is one level only; parent cells are not destroyed upon refinement; algorithms of automatic generation and destruction of refined cells are implemented. The below given are two examples of using a refined grid.

Problem 4. A cylinder impact on a rigid wall. The initial problem geometry and initial computational grid are shown in Fig.9a. In the region occupied by the cylinder, the grid used for computations was refined up to the 2-nd level. Computations were carried out in elastic-plastic approximation, their results are shown in Figs.9b and 9c. The computation speedup ratio was ~6.5 with the use of the refined grid.



a)



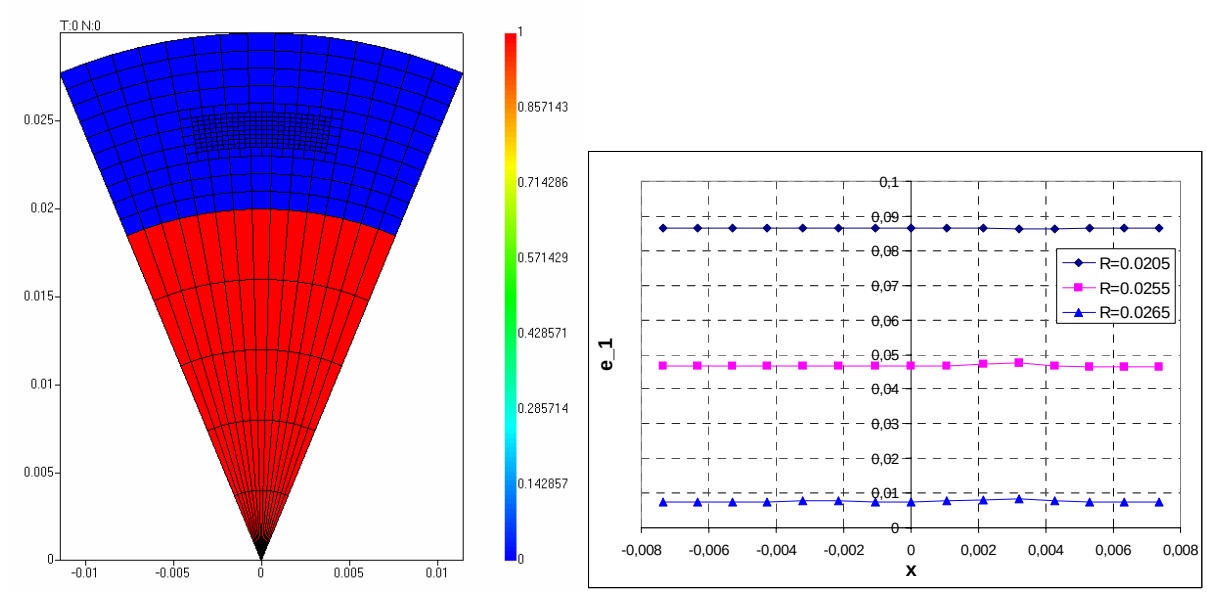
b) **c)**

Figure 9. A cylinder impact on a rigid wall

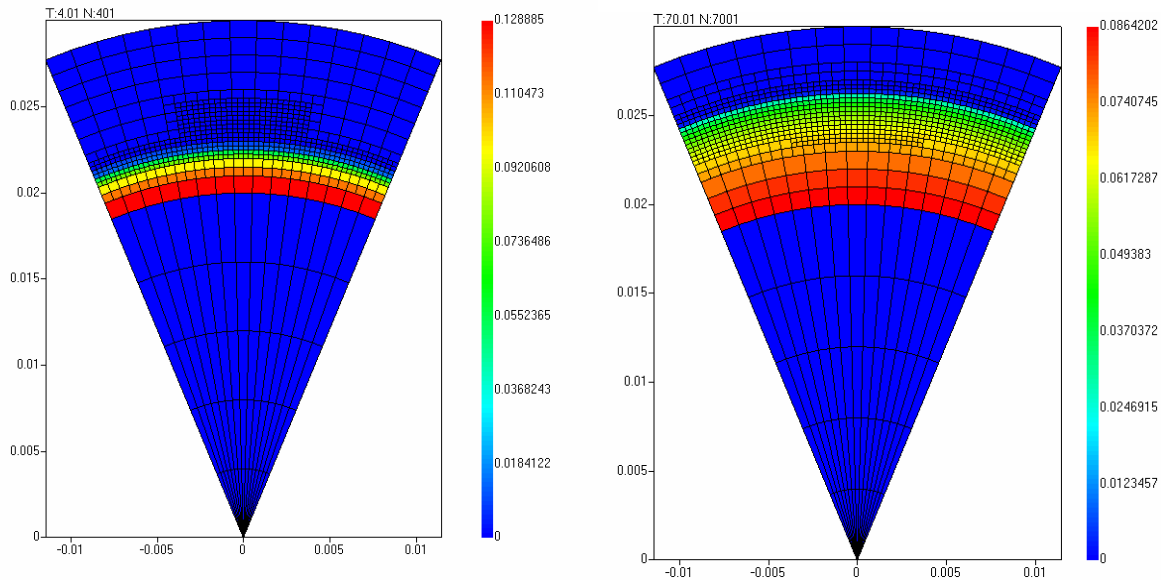
Problem 5. Propagation of heat wave.

A spherically symmetric problem is considered. There are two regions filled with various materials. In the first region ($R<R_1=0.02$), there is an ideal gas with $\gamma = 5/3$ and initial parameters $\rho_1 = 1.0$, $e_1 = 1.0$. The second region ($R_1 \le R \le R_2=0.03$) contains a material of $\rho_2 = 5.0$, $e_2 = 0.0$ and with Mie-Grueneisen EOS. The initial geometry of the problem and the initial grid are shown in Fig.10a. The grid remains unchanged during computations. Besides, a refined grid of the second level is specified and maintained on the heat wave front during the computational process.

Results of this computation are given in Figs.10c-d in the form of a raster picture of energy of one of the materials and a computational grid at two time points.



a) b)



c) d)

Figure 10. Propagation of a spherically symmetric heat wave

Figure 10b shows plots of energy dependences in the first material along axis OX for three rows of the reference grid. The heat wave front at the given time corresponds to radius R=0.0265. R=0.0205 corresponds to cells located before the stable-state refinement region, R=0.0255 corresponds to cells located behind the stable-state refinement region in the direction of heat propagation. One can see from these figures that if a stable-state grid at the region center is used in combination with a mobile refined grid on the wave font, the flow symmetry actually appears to be not distorted.

Parallelization Specifics in TREK Technique

In the approach used to construct a parallel code the key point is irregular point-to-point parallelization, in which calculations of quantities determined at one point are and elementary indivisible work units. One processor executes calculations for an absolutely random set of points. Fig.11 shows the example of problem decomposition over processors for a 2D cross section. The set of computation points and the order of calculations are determined by special control lists. The computational program is always arranged as a loop in the control list of points. The loop implementation provides for a possibility to interrupt calculations in order to perform interpocessor communications, with the data from one layer of cells being transmitted from one processor to another. Inside the loop, calculations for one computational cell of a random number are programmed. The point number is given from the control list of the numbers of points. The program arrangement admits dynamic changes of control lists on each processor. Such approach allows:

1. arbitrarily varying the distribution of points over processors;
2. calculations up to one point and “pasting in” communications among calculations at points;
3. dividing the computational module programming into a program for control of the order of calculations and communications and the program for calculation at one computational point of the given number.

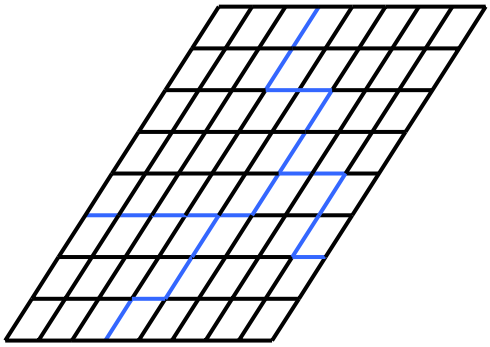


Figure 11. Example of the problem decomposition over processors.

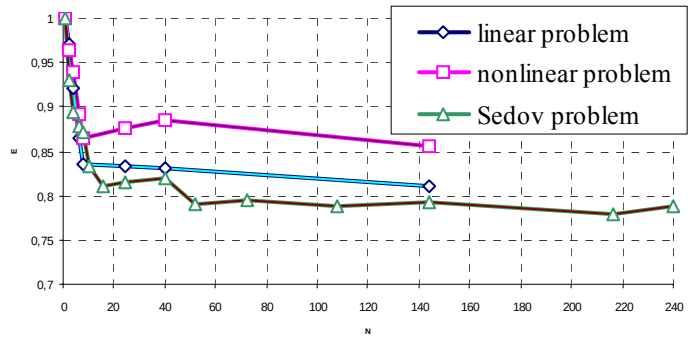


Figure 12. Measurements of the efficiency for problems 6 and 7.

Problem 6. Measurement of the gas dynamics parallelization efficiency.

Within the entire computational region 1 (0<X<10.5, 0<Y<10.5, 0<Z<10.5) there is an ideal gas (ρ_1=1, e_1=0, u_1=0, γ=1.4), in region 2 (0<X<1, 0<Y<1, 0<Z<1) energy e_2= 1 is specified. The number of cells per processor remained unchanged in all computations and was equal to 105*105*105 cells. Measurement results are shown in Fig.12.

Thus, for the gas dynamics problem the efficiency of parallel computations was about 0.8 in the problem multiplication mode.

Problem 7. Measurements of the efficiency of heat transfer parallelization.

The linear and nonlinear problems of the propagating spatial heat wave are considered. As in the computations described above, the number of cells per processor was 105*105*105 in all computations. Measurement results are shown in Fig.12. The efficiency of parallel computations for the heat transfer problem was not less than 0.8 in the linear problem and 0.85 in the nonlinear problem.

For a more detailed description of the methods of TREK prallelization see the paper by Belyaev, 2000.

Conclusion

The paper presents some innovations to EGAK and TREK techniques aimed at improvement of the accuracy and efficiency of computations. Results of some test computations giving a notion of capabilities of these techniques for simulation of multi-material flows with large deformations are presented.

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