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The Discontinuous Galerkin Method and its Implementation in the RAMEG3D Software Package

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Abstract

Currently, the Discontinuous Galerkin Method (DGM) is widely used to solve complex multi-scale problems of mathematical physics that have important applied significance. When implementing it, the question of choosing a discrete approximation of flows for viscous terms of the Navier-Stokes equation is important.

It is necessary to focus on the construction of limiting functions, on the selection of the best discrete approximations of diffusion flows, and on the use of implicit and iterative methods for solving the obtained differential-difference equations for the successful application of DGM on three-dimensional unstructured grids.

First-order numerical schemes and second-order DGM schemes with Godunov, HLLC, Rusanov-Lax-Friedrichs numerical flows and hybrid flows are investigated. For high-order precision methods, it is necessary to use high-order time schemes. The Runge-Kutta scheme of the third order is used in the work. The equations are written as a system of first-order equations, when solving the Navier-Stokes equation by the discontinuous Galerkin method.

Keywords: Discontinuous Galerkin Method (DGM), Navier-Stokes equations, hybrid flows, Runge-Kutta scheme, scheme template.

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Обзорная статья

Разрывный метод Галеркина и его реализация в программном комплексе РАМЕГ3D

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Аннотация

В настоящее время метод Галеркина с разрывными базисными функциями (РМГ) или *Discontinuous Galerkin Method* (DGM) получил широкое распространение для решения сложных разномасштабных задач математической физики, имеющих важное прикладное значение. При его реализации важным является вопрос о выборе дискретной аппроксимации потоков для вязких членов уравнения Навье-Стокса.

Для успешного применения РМГ на трехмерных неструктурированных сетках необходимо сосредоточить внимание на построении лимитирующих функций, на выборе наилучших дискретных аппроксимаций

диффузионных потоков и на применении неявных и итерационных методов решения полученных дифференциально-разностных уравнений.

Исследуются численные схемы первого порядка и схемы РМГ второго порядка с численными потоками Годунова, HLLC, Русанова-Лакса-Фридрихса и гибридными потоками. Для методов высокого порядка точности необходимо использовать схемы высокого порядка по времени.

В работе используется схема Рунге-Кутты третьего порядка. При решении уравнения Навье-Стокса разрывным методом Галеркина уравнения записываются в виде системы уравнений первого порядка.

Ключевые слова: разрывный метод Галеркина, уравнения Навье-Стокса, гибридные потоки, схема Рунге-Кутты, шаблон схемы.

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One of the main requirements is the use of high-precision numerical methods to obtain high-quality solutions to mathematical physics problems of important applied importance, one of the main requirements is the use of high-precision numerical methods. This is especially relevant for solving complex multi-scale problems in which it is not enough to obtain a solution only by grinding the grid and using first-order accuracy methods.

The *Discontinuous Galerkin Method* (DGM) has been developing especially actively over the past few decades, the first mention of which can be found in [1]. This method refers to numerical methods of an increased order of approximation of the solution, because it provides a given order of accuracy, and on unstructured grids, can be used for grids with an arbitrary cell shape, has a compact template consisting of a calculated cell and one layer of neighboring cells. There are two approaches to improve the accuracy of the resulting solution. One of them is the shredding of the grid in the areas of the existing features of the solution, the second approach is to increase the order of accuracy of the scheme. The use of the discontinuous Galerkin method makes it possible to use both approaches at once: increasing the order of accuracy of the method by increasing the order of the polynomials used, and local grinding of the grid (the so-called *hp*-adaptation) [2, 3].

One of the important issues in the implementation of the method is the choice of the grid on which the solution is being sought. The undoubted advantage of RMG is the possibility of its application on grids of arbitrary structure. Currently, the discontinuous Galerkin method is well developed for both structured [4] and unstructured [5] grids. There are successful DGM software implementations for solving three-dimensional problems on unstructured grids containing elements of only one type (tetrahedral [5–8] or hexahedral [9]), as well as for grids of arbitrary structure [10].

The obvious disadvantage of the method is its extremely high computational cost, but this is covered by a compact template and the creation of efficient parallel software systems. DGM has a significant computational complexity, so the question arises about the most efficient use of all the possibilities of computer technology. In the world research centers dealing with this problem, work is underway to parallelize the implementations of DGM on a super computer [11–13]. In [6], when solving the Navier-Stokes DGM equations, a new grid-operator approach to programming mathematical physics problems was used, which allows to compactly record and effectively apply mathematical formulas, uniformly implement the approach on different types of grids and for various computing architectures, including for CUDA graphics accelerators [14, 15].

Along with the many advantages of using the discontinuous Galerkin method, there are also some difficulties in its implementation. Firstly, in order to ensure the monotony of the solution obtained by this method, it is necessary to introduce slope limiters or limiters, especially if the solution contains strong discontinuities. The most widely used is the Cockburn limiter [16]. The idea of this limiter is easily implemented in the multidimensional case on grids of arbitrary structure. However, this limiter, like all TVD limiters, reduces the accuracy of the resulting solution. Recently, various approaches to solving this problem have been actively developing. One of the approaches to creating a limiter of an increased order of accuracy is proposed in the works of Krivodanova [17]. But this limiter works well only on structured grids. Other approaches to creating limiters of a higher order of accuracy are described in [18–25].

Also important in the implementation of DGM is the question of choosing a discrete approximation of flows for viscous terms of the Navier-Stokes equation. There are several types of such approximations, most often used in real calculations [26, 27], which were investigated in [28]. Nevertheless, the question of the optimal choice of such approximations remains open.

When the order of accuracy of the scheme increases, there is a strict restriction on the time step. Initially, when calculating DGM, time integration was carried out by explicit multistep Runge-Kutta schemes of high order [16, 29, 30]. But the most effective approach is to use implicit time integration methods in order to relax the time step constraint [31–36].

Currently, software implementations of DGM are known by an implicit method for modeling incompressible flows [37] and for solving the Navier-Stokes equations [35].

Another point that the authors had to face when implementing DGM on grids with an arbitrary cell shape is the need to carry out the integration procedure [16] on an arbitrary cell shape. To do this, the transformation of the original irregular-shaped cell into a reference cell for which the position of the quadrature points is known [61]. When constructing such a transformation for the case of a tetrahedron, hexahedron and triangular prism, it is sufficient to use a multilinear transformation that translates the vertices of the cell into the vertices of the original cell. However, for a quadrangular pyramid, this approach does not give the desired result, because when using it, we get curved side faces and edges of the pyramid, which will not allow it to be properly joined with tetrahedral cells. Below in this paper, a transformation is constructed that avoids this drawback.

For the successful implementation of DGM on three-dimensional unstructured grids, it is necessary to focus on several points:

- on the construction of limiting functions;
- on the selection of the best discrete approximations of diffusion flows;
- on the application of implicit and iterative methods for solving the obtained differential-difference equations.

To obtain an accurate numerical solution of mathematical physics problems, it is important to use a high-quality computational grid and a reliable high-precision numerical method, as well as to be sure that the chosen method fully corresponds to the problem being solved. For example, it is known that when using Godunov-type difference schemes in some problems containing shock waves, the development of instability of the “carbuncle” type occurs [38, 39]. The conditions for the appearance of this type of instability are high Reynolds numbers and a low dissipative numerical flow. It was noted in [40] that other types of instabilities may occur under such conditions. One of the established causes of this type of instability is the numerical flows used [41–48]. Flows with low dissipation are most susceptible to the occurrence of this instability, and the use of highly dissipative flows allows avoiding the occurrence of “carbuncle” instability. For this reason, several attempts have been made to develop new methods that suppress the development of instabilities, ensuring low dissipation [49–52]. In [53], a study of the susceptibility to shock-wave instability of specific numerical flows implemented in the RAMEG3D software package was carried out [54]. This type of instability is tested on test problems from the Kerk list [40] in the statements given in [55].

In this paper, we study first-order numerical schemes and second-order DGM schemes with numerical Godunov flows [56], HLLC [57], Rusanov-Lax-Friedrichs flows [58, 59] and hybrid flows [60] used in calculations. The basic formulas of the hybrid flow developed by the authors are also given.

1. Basic formulas of the discontinuous Galerkin method. Consider the Navier-Stokes equations written as a system of first-order equations:

$$\begin{aligned}\partial_t U + \nabla \cdot F(U) - \nabla \cdot G(U, \tau) &= 0, \\ \tau &= \left(\lambda - \frac{2}{3} \mu \right) \hat{E}(\operatorname{div} v) + 2\mu S(v), \\ S(v) &= \frac{1}{2} \left(\nabla v + (\nabla v)^* \right), \\ q(U) &= k \nabla T.\end{aligned}\tag{1}$$

$$\begin{aligned} U &= (\rho, \rho u, \rho v, \rho w, E), \\ F(U) &= (F_x(U), F_y(U), F_z(U)), \\ G(U, \tau) &= (G_x(U, \tau), G_y(U, \tau), G_z(U, \tau)). \end{aligned} \quad (2)$$

$$\begin{aligned} F_x(U) &= (\rho u, \rho u^2 + p, \rho uv, \rho uw, (E + p)u), \\ F_y(U) &= (\rho u, \rho uv, \rho v^2 + p, \rho vw, (E + p)v), \\ F_z(U) &= (\rho u, \rho vw, \rho vw, \rho w^2 + p, (E + p)w), \\ G_x(U, \tau) &= (0, \tau_{xx}, \tau_{xy}, \tau_{xz}, u\tau_{xx} + v\tau_{xy} + w\tau_{xz} + q_x), \\ G_y(U, \tau) &= (0, \tau_{yx}, \tau_{yy}, \tau_{yz}, u\tau_{yx} + v\tau_{yy} + w\tau_{yz} + q_y), \\ G_z(U, \tau) &= (0, \tau_{zx}, \tau_{zy}, \tau_{zz}, u\tau_{zx} + v\tau_{zy} + w\tau_{zz} + q_z), \end{aligned} \quad (3)$$

where ρ is the substance density; u, v, w are the velocity components v, ε is the specific internal energy and $E = \rho \left(\varepsilon + \frac{u^2 + v^2 + w^2}{2} \right)$ is the total energy per unit volume, p is the substance pressure.

The system of equations (1) is closed by the equation of state, in this case, the equation of state of an ideal gas $p = (\gamma - 1)\rho\varepsilon$ with an adiabatic exponent γ .

For each specific task, system (1) is supplemented with suitable initial-boundary conditions.

Let's cover the area Ω , where the solution is sought by the discontinuous Galerkin method with a grid T_h . On each element T_j we will look for an approximate solution of the system of equations (1) in the form of polynomials $P(x)$ of degree N with time-dependent coefficients [1]:

$$\begin{aligned} U_h(x, t) &= \sum_{k=0}^{st} U_k(t) \phi_k(x), \\ q_{ih}(x, t) &= \sum_{k=0}^{st} q_{ik}(t) \phi_k(x), \\ \tau_{ijh}(x, t) &= \sum_{k=0}^{st} \tau_{ijk}(t) \phi_k(x), i, j = x, y, z, \end{aligned} \quad (4)$$

where $st = 0, C_{N+3}^3 - 1$ is the dimension of the polynomial space, and $\phi_k(x)$ is the basis function.

For high-order precision methods, it is necessary to use high-order time schemes. In this paper, the Runge-Kutta scheme of the third order is used [1].

The equations are written as a system of first-order equations, and the solution occurs in two stages when solving the Navier-Stokes equation by the discontinuous Galerkin method. At the first stage, the components of the temperature gradient and the viscous stress tensor are calculated. Their approximation, as well as the approximation of the solution, within the grid cell when implementing the modal approach is in the form of polynomials of degree p with time-dependent coefficients. At the boundary of the element, the flow values of the quantities are determined by some rule from the values inside the element and from the values in the cell adjacent to this element.

At the second stage, the components of the vector of conservative variables are determined. In this case, convective flows can be calculated using various variants of the exact or approximate solution of the Riemann problem. Diffusion flows at the element boundary can also be calculated in various ways, a detailed analysis of which was carried out in [63]. Quadrature formulas of the required order are used to calculate integrals. This two-step approach allows us to calculate gradients with the same order of accuracy as conservative variables, while maintaining the compactness of the scheme template.

2. Hybrid flow's building. In [60], a hybrid numerical flow was constructed, the main idea of which was proposed in [52]. This flow is a linear combination of one of the flows (HLLC or Godunov flow) and a stable Rusanov-Lax-Friedrichs flow (RLF).

The direction of the velocity jump determines the normal to the shock wave: when the cell boundary coincides with the shock wave front, the Godunov flow ($\mathbf{F}^{\text{Godunov}}$), is used, and when the interface is perpendicular to the shock wave, the Rusanov-Lax-Friedrichs flow ($\mathbf{F}^{\text{RLF}}$) is applied. Thus, dissipation increases in the direction coinciding with the shock wave, and instability is eliminated:

$$\hat{\mathbf{F}} = \theta \mathbf{F}^{HLLC} + (1 - \theta) \mathbf{F}^{RLF}, \quad (5)$$

$$\hat{\mathbf{F}} = \theta \mathbf{F}^{\text{Godunov}} + (1 - \theta) \mathbf{F}^{RLF}, \quad (6)$$

$$\text{where } \theta = \begin{cases} \frac{|\Delta \mathbf{u} \cdot \mathbf{n}|}{|\Delta \mathbf{u}|} = \frac{|\Delta u n_x + \Delta v n_y + \Delta w n_z|}{\sqrt{\Delta u^2 + \Delta v^2 + \Delta w^2}}, & |\Delta \mathbf{u}| > \varepsilon, \\ 1, & |\Delta \mathbf{u}| \leq \varepsilon, \end{cases} \quad (7)$$

where ε is a small constant to avoid division by zero (for example $\varepsilon = 10^{-6}$); $\mathbf{n}$ is the normal to the cell boundary, and $\Delta \mathbf{u} = (u_L - u_R, v_L - v_R, w_L - w_R)$ is the jump of the velocity vector across the boundary. The parameter θ is calculated from the normal to the cell boundary and the velocity jump through the cell boundary surface.

Another approach to the construction of a hybrid flow is to add a dissipative term in the areas where it is necessary.

To construct it, we will switch to a local coordinate system with an ort $(\mathbf{n}, \boldsymbol{\tau}_1, \boldsymbol{\tau}_2)$, where $\mathbf{n}$ is the vector of the external normal to the surface through which the flow is considered; $\boldsymbol{\tau}_1, \boldsymbol{\tau}_2$ any single orthogonal vectors lying on this surface. Vectors $\mathbf{U}$ and $\mathbf{F}$ in this coordinate system (indicated by the index $*$) will have the form:

$$\begin{aligned} \mathbf{U}^* &= (\rho, \rho(\mathbf{u}, \mathbf{n}), \rho(\mathbf{u}, \boldsymbol{\tau}_1), \rho(\mathbf{u}, \boldsymbol{\tau}_2), E)^T, \\ \mathbf{F}^*(\mathbf{U}) &= (\rho(\mathbf{u}, \mathbf{n}), \rho(\mathbf{u}, \mathbf{n})u_n + p, \rho(\mathbf{u}, \mathbf{n})u_{\tau_1}, \rho(\mathbf{u}, \mathbf{n})u_{\tau_2}, (E + p)(\mathbf{u}, \mathbf{n})). \end{aligned} \quad (8)$$

In order to obtain a new flow with greater dissipation than the Godunov flow (HLLC) and less dissipation than the RLF flow, we choose a certain velocity W in the original coordinate system and switch to an inertial frame of reference moving at this speed.

Let's denote the maximum velocity $W_{\max}$, the minimum velocity — $W_{\min}$ (taking into account the sign) of the waves generated during the decay of an arbitrary discontinuity in the case of using the Godunov flow (or using the HLLC flow). Note that if W is greater than $W_{\max}$, then the values of the gas-dynamic quantities will coincide with U^+ and after recalculation to the original coordinate system, this flow will be equal, respectively, to use the Godunov flow and the HLLC flow:

$$\begin{aligned} \hat{\mathbf{F}} &= \mathbf{F}^{\text{Godunov}}(\mathbf{U}^{*+}) - W \mathbf{U}^{*+}, \\ \hat{\mathbf{F}} &= \mathbf{F}^{\text{HLLC}}(\mathbf{U}^{*+}) - W \mathbf{U}^{*+}. \end{aligned}$$

Accordingly, if $-W$ is less than $W_{\min}$, then the values of the gas-dynamic quantities will coincide with U^- , and after recalculation to the original coordinate system, this flow will be equal to:

$$\begin{aligned} \hat{\mathbf{F}} &= \mathbf{F}^{\text{Godunov}}(\mathbf{U}^{*-}) + W \mathbf{U}^{*-}, \\ \hat{\mathbf{F}} &= \mathbf{F}^{\text{HLLC}}(\mathbf{U}^{*-}) + W \mathbf{U}^{*-}. \end{aligned}$$

Taking the half-sum of these streams, we get the RLF stream. If $W=0$, then, respectively, Godunov flows (or HLLC) are obtained.

Thus, if $0 < W < W_{\max}^*$, where $W_{\max}^* = \max(|W_{\max}|, |W_{\min}|)$ get a new flow, the average between the Godunov flow (HLLC) and the RLF flow and having greater dissipation than the Godunov flow (HLLC) and less dissipation than the RLF flow. This type of flow was considered in [62].

The hybrid stream used can be obtained as follows. Consider an inertial coordinate system moving at a speed $W \cdot \mathbf{n}$ relative to the original system, and calculate the Godunov flux or HLLC, which we then recalculate in the original coordinate system (Fig. 1). The resulting value is denoted by $\mathbf{U}^{*+}$. We will carry out a similar procedure with speed $-W \cdot \mathbf{n}$ and denote the corresponding value $\mathbf{U}^{*-}$. Taking a half-sum of such flows, we come to the formulas:

$$\hat{\mathbf{F}} = \frac{\mathbf{F}^{\text{Godunov}}(\mathbf{U}^{*+}) + \mathbf{F}^{\text{Godunov}}(\mathbf{U}^{*-})}{2} - W \frac{\mathbf{U}^{*+} + \mathbf{U}^{*-}}{2}, \quad (9)$$

$$\hat{\mathbf{F}} = \frac{\mathbf{F}^{\text{HLLC}}(\mathbf{U}^{*+}) + \mathbf{F}^{\text{HLLC}}(\mathbf{U}^{*-})}{2} - W \frac{\mathbf{U}^{*+} + \mathbf{U}^{*-}}{2}, \quad (10)$$

$$W = \theta W^*, \quad W^* = \max(|u+c|, |u-c|), \quad (11)$$

$$\theta = \begin{cases} M \leq M_{\min}, & W = W^*, \\ M_{\min} < M < M_{\max}, & W = \frac{M_{\max} - M}{M_{\max} - M_{\min}} W^*, \\ M \geq M_{\max}, & W = 0, \end{cases} \quad (12)$$

where W^* is the maximum of the modules of the eigenvalues of the matrix $\frac{\partial \mathbf{F}^*(U)}{\partial U^*}$; θ is the parameter [52].

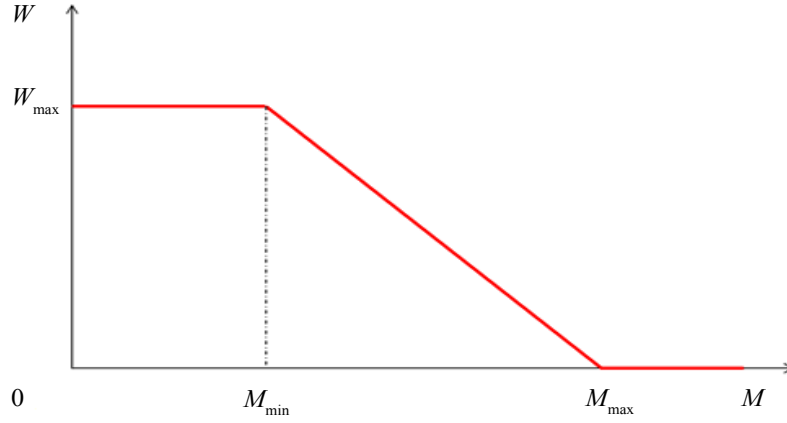


Fig. 1. The constructed hybrid flow, the average between the Godunov flow (HLLC) and the RLF flow

3. Numerical integration on arbitrary cells. Consider the transformation of an arbitrary quadrangular pyramid P with vertices (x_i, y_i, z_i) $i = 1, 5$ in the coordinate system $OXYZ$ into a regular quadrangular pyramid P with vertices $(0,0,0)$, $(1,0,0)$, $(0,1,0)$, $(1,1,0)$, $(0.5,0.5,1)$ in the coordinate system $O\alpha\beta\gamma$ (Fig. 2). The base of the pyramid P will be translated into the base of the pyramid P^* using a bilinear transformation:

$$\begin{aligned} x &= a_0 + a_1\alpha + a_2\beta + a_3\alpha\beta, \\ y &= b_0 + b_1\alpha + b_2\beta + b_3\alpha\beta, \\ z &= c_0 + c_1\alpha + c_2\beta + c_3\alpha\beta, \end{aligned} \quad (13)$$

where the coefficients $a_i, b_i, c_i, i = \overline{0,3}$ are defined explicitly:

$$a_0 = x_1, a_1 = x_2 - x_1, a_2 = x_3 - x_1, a_3 = x_4 - x_3 - x_2 + x_1.$$

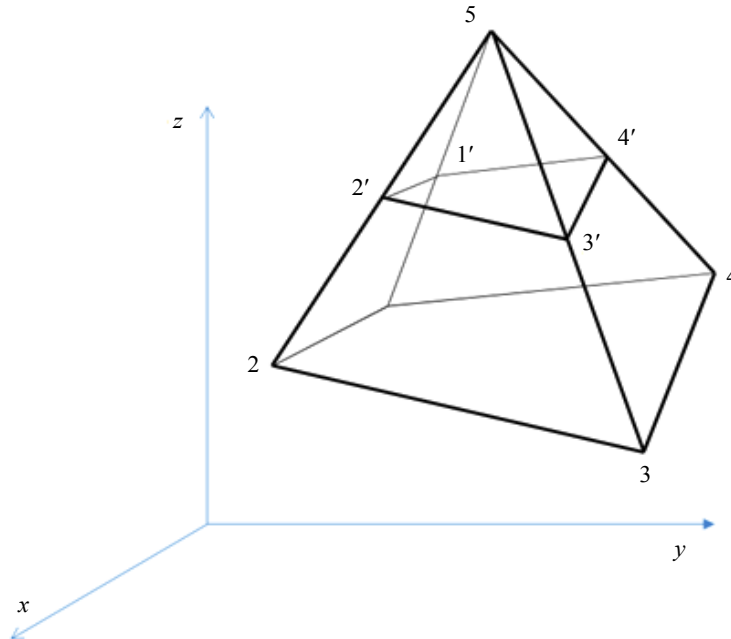


Fig. 2. An arbitrary quadrangular pyramid in space

Let's build an arbitrary pyramid P' with a vertex at point 5 (Fig. 3) and a base with vertices at points 1'–4', by compressing the original pyramid.

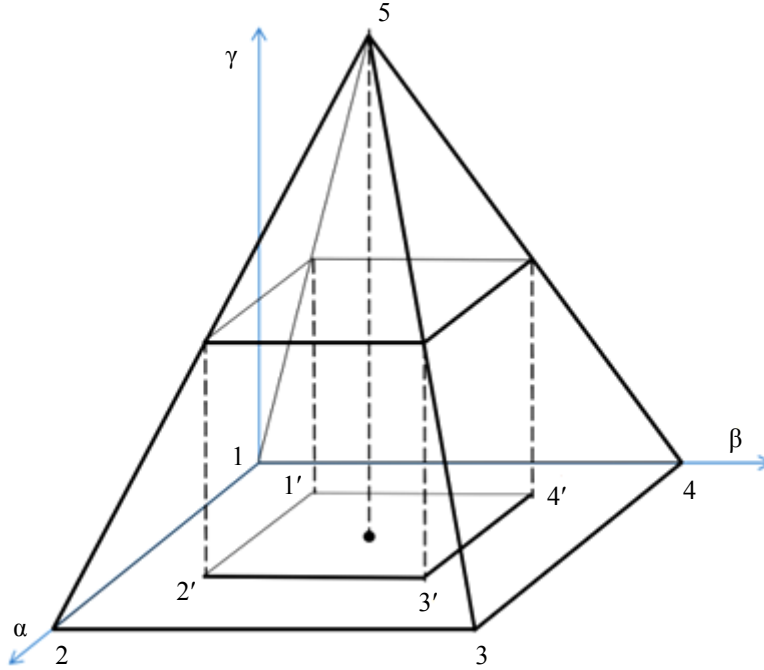


Fig. 3. A regular quadrangular pyramid

The coordinates x'_i can be defined as:

$$\begin{cases} x'_1 = x_1(1-\gamma) + x_5\gamma, \\ x'_2 = x_2(1-\gamma) + x_5\gamma, \\ x'_3 = x_3(1-\gamma) + x_5\gamma, \\ x'_4 = x_4(1-\gamma) + x_5\gamma, \end{cases} \quad (14)$$

where $\gamma \in [0, 1]$ is the compression ratio.

Let's make a similar transformation in the reference pyramid with the same compression ratio. The resulting base of the compressed pyramid will be transferred to the base of the reference pyramid. The coordinates of these points in the coordinate system $0\alpha\beta$ are equal to:

$$\begin{aligned} 1' &\rightarrow \alpha = \frac{\gamma}{2}, \beta = \frac{\gamma}{2}, \\ 2' &\rightarrow \alpha = 1 - \frac{\gamma}{2}, \beta = \frac{\gamma}{2}, \\ 3' &\rightarrow \alpha = 1 - \frac{\gamma}{2}, \beta = 1 - \frac{\gamma}{2}, \\ 4' &\rightarrow \alpha = \frac{\gamma}{2}, \beta = 1 - \frac{\gamma}{2}. \end{aligned} \quad (15)$$

Using the transformation (13)–(15), the coordinates of the points x'_i are:

$$\begin{cases} x'_1 = a_0 + a_1 \frac{\gamma}{2} + a_2 \frac{\gamma}{2} + a_3 \frac{\gamma^2}{4} = x_1(1-\gamma) + x_5\gamma, \\ x'_2 = a_0 + a_1 \left(1 - \frac{\gamma}{2}\right) + a_2 \frac{\gamma}{2} + a_3 \left(1 - \frac{\gamma}{2}\right) \frac{\gamma}{2} = x_2(1-\gamma) + x_5\gamma, \\ x'_3 = a_0 + a_1 \left(1 - \frac{\gamma}{2}\right) + a_2 \left(1 - \frac{\gamma}{2}\right) + a_3 \left(1 - \frac{\gamma}{2}\right)^2 = x_3(1-\gamma) + x_5\gamma, \\ x'_4 = a_0 + a_1 \frac{\gamma}{2} + a_2 \left(1 - \frac{\gamma}{2}\right) + a_3 \left(1 - \frac{\gamma}{2}\right) \frac{\gamma}{2} = x_4(1-\gamma) + x_5\gamma. \end{cases} \quad (16)$$

Solving this system of equations (16), the conversion coefficients (13) are:

$$a_3 = \frac{x_4 - x_2 - x_3 + x_1}{1 - \gamma},$$

$$a_1 = (x_2 - x_1) - \frac{\gamma}{2(1 - \gamma)}(x_4 - x_2 - x_3 + x_1),$$

$$a_2 = (x_3 - x_1) - \frac{\gamma}{2(1 - \gamma)}(x_4 - x_2 - x_3 + x_1),$$

$$a_0 = \frac{x_1 + x_2 + x_3 + x_4}{4}(1 - \gamma) + \gamma x_5 - \frac{x_2 - 2x_1 + x_3}{2} + \frac{2\gamma - 1}{4(1 - \gamma)}(x_4 - x_2 - x_3 + x_1).$$

As a result, get the transformation for the coordinate x :

$$x = \frac{x_1 + x_2 + x_3 + x_4}{4}(1 - \gamma) + \gamma x_5 - \frac{x_2 - 2x_1 + x_3}{2} + \frac{2\gamma - 1}{4(1 - \gamma)}(x_4 - x_2 - x_3 + x_1) +$$

$$+ \left[(x_2 - x_1) - \frac{\gamma}{2(1 - \gamma)}(x_4 - x_2 - x_3 + x_1) \right] \alpha +$$

$$+ \left[(x_4 - x_1) - \frac{\gamma}{2(1 - \gamma)}(x_4 - x_2 - x_3 + x_1) \right] \beta +$$

$$+ \left[\frac{x_4 - x_2 - x_3 + x_1}{1 - \gamma} \right] \alpha \beta.$$

Similarly, transformation for the y, z coordinates is obtained.

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