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INFLUENCE OF NUMERICAL DIFFUSION ON EXACTNESS OF CALCULATION IN SOFTWARE FLUENT

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Abstract: *Numerical diffusion impairs the exactness of discrete solutions of the equations governing the convective transport of a scalar when the flow is not aligned with grid lines. Numerical diffusion leads to unintentional smoothing of adverted gradients. This work presents an assessment of numerical diffusion in CFD code FLUENT 6.3 and available means of reducing impairment.*

Key words: *numerical diffusion, grid, Fluent.*

1. Introduction

The solution of transport equations in Fluent utilizes of discretionary process, where basic problem is exact calculation of transport parameter Φ through walls of specific volume and his convective flow through these boundaries. It is necessary to compute with existence "false" numerical diffusion and also with occurrence discretionary values Φ, which they are outside of the region of correct solution. This paper compares physical exactness of computation by using offered discretionary schemas, which they are designed in CFD code in Fluent 6.3 and possibility to reduce this numerical errors.

The software Fluent utilizes the finite volumes method to transfer (numerically) of general transportation equations to the system of linear equations by using the Gauss-Seidl iteration method. This process consist of integrating of equations at each control volume - cell. The results are the discretionary equations, which present the stability of flow, it is the laws of conservation every transport parameter Φ in a given volume. In this paper is demonstrated the discretionary equations at a law of preservation to transport parameter Φ by stationary flow, which can describe by equation in integrating shape (1). The equation (1) presents the balance of flow in constant volume [5], [6]:

$$\int_A \rho \vec{v} \cdot \mathrm{d}\vec{A} = \int_A \Gamma_\Phi \nabla\Phi \cdot \mathrm{d}\vec{A} + \int_V S_\Phi \,\mathrm{d}V\,, \qquad (1)$$

where: ρ - is density; $\vec{v}$ is vector of velocity; $\vec{A}$ - is vector of region; Γ_Φ - is diffusion coefficient of parameter Φ; ∇Φ - is gradient of parameter Φ; S_Φ - is source parameter Φ at a unit of volume [1-4].

The equation (1) was applied at all control volumes (cells) of computing regions.

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We can get after the discretionary of equations (1) in cell:

$$\sum_{f}^{N_{faces}} \rho_f \vec{v}_f \Phi_f \vec{A}_f = \sum_{f}^{N_{faces}} \Gamma_\Phi \nabla\Phi_f \vec{A}_f + S_\Phi V, \quad (2)$$

where: N_{faces} - is number of walls (faces) surrounded of cell; Φ_f - is value of parameter Φ flowed during region f; $\rho_f \vec{v}_f \vec{A}_f$ - is weighted flow through surface; $\vec{A}_f$ - is vector of surface f; $\nabla\Phi_f$ - is gradient of parameter Φ per surface f; V - is volume of cell.

Left sides of equations (1) and (2) introduce the convective transfer of parameter Φ, right sides introduce diffusive transfer and source member of the transport parameter Φ (it is reduction alternatively rising). Basic problem at discretionary of convective member is exact computing of transport parameter on the wall of specific volume Φ_f and its gradient $\nabla\Phi_f$. The diffusion process influences transfer of transport parameter along its gradient in all directions. The convective transfer radiates only in direction of flows. It is very difficult to find exact discretionary of computing scheme by solving of convective member in the equation (2).

The numerical diffusion comes into being mainly in example, when the direction of flow isn't parallel with walls of grid. This optimal status (parallel flow) can be obtained only by computations of direct sectors of pipes without barriers by using hexa cells. The direction of flow (at mostly example) is respected in general direction of cell's walls (hexa, tetra, polyhedra). It is necessary to expect a numerical error by evaluating the solutions.

The equation (2) contains unknown the scalar parameter Φ in centre of cell and together unknown the scalar values Φ_{nb} in nearby cells. The equation is generally non-linear and after that the equation is transformed to linear form:

$$a_P \Phi = \sum_{nb} a_{nb} \Phi_{nb} + b. \quad (3)$$

Index *nb* represents contiguous (surrounding) cells, a_p and a_{nb} are linearized coefficients for parameter Φ and Φ_{bn}.

Number of surrounding cells depends on typology of grid, but a number of cells are given by number of walls created of solved cell in most of solved examples. The equation (3) describes a status into all cells of grid. The system of linear equations was solved to implicitly by using the Gauss-Seidl method with combination to algebraically „multidrid" multistage method, it is AMG in Fluent.

The software Fluent is saving discreet values of scalar parameter Φ in centre of cell. Values of scalar parameters Φ_f are required on walls of cells for calculation of convective member (left side of equation) too. The value s of scalar parameters Φ_f are specified by interpolation from values in centre of contiguous of surrounding cells. There is used „upwind" scheme in this process, it is seen the value Φ_f is derived from value of following cell in direction of flow.

The software Fluent was allowed to choose from five "upwind" schemes for computation of convective member: First-order upwind, Power-law, Second-order upwind, Quick, Third-order Muscl, but Quick schema could be used only for hexa cells.

The diffusion member in equation (2) (first member at a right side) is setting in a "Central-differencing" computing scheme of second order, which is satisfactory exact.

It is necessary to determinate gradients by solution of flow, but for discretization of convective and diffusion member in equation (2) too. The gradients are needed for computation of values of scalar parameters on walls of cells. The gradient $\nabla\Phi$ could be computed by three ways: Green-Gauss Cell-Based, Green-Gauss Node-Based and Least Squares Cell-Based. Calculation of gradient by way: Least Squares Cell-Based is recommended for polyhedra cells [4].

The Green-Gaus theorems computes gradient in centre of cell in form:

$$(\nabla\Phi)_{c0} = \frac{1}{V}\sum_f \overline{\Phi}_f \vec{A}\,, \tag{4}$$

whereby value of cell on wall Φ_f was computed by Green-Gauss Cell-Based method as mean value from values of nearby cells:

$$\overline{\Phi}_f = \frac{\Phi_{c0} + \Phi_{c1}}{2}\,, \tag{5}$$

whereas value of cell is computed by using Green-Gauss Cell-Based method as mean value from nodes of given wall:

$$\overline{\Phi}_f = \frac{1}{N_f}\sum_n^{N_f} \overline{\Phi}_n\,, \tag{6}$$

N_f is number of nodes.

The value in node $\overline{\Phi}_n$ was computed from values in centre all cells with given node.

2. Description of Tested Job

The goal of testing examples was the interpretation of degrees of physical exactness of numerical calculation in dependence not only at a density and shape grid, but at a choice of computational schemes and the accesses to the calculations of gradients of transportation parameter too.

It was simulated 3D stationary flow of fictional gas, where density is $\rho = 1$ kgm^{-3}, in the computing region of dimensions 1x1x0.2 m (Figure 1). The values of thermal conductivity λ [Wm^{-1}K^{-1}] and dynamic viscosity μ [Pas] of gas is gone near the zero. The boundary conditions are introduced in Table 1.

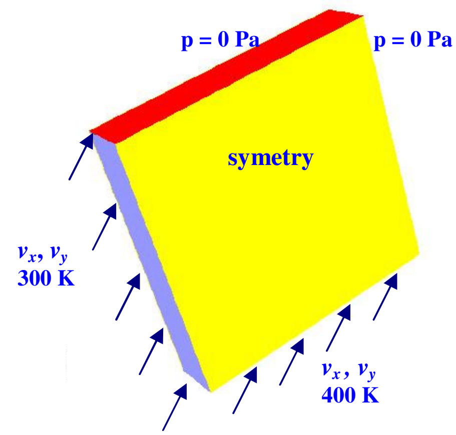


Fig. 1. *Schema of computed region 1x1x0.2 m*

The object of observation was specified the levels of dispersion (numerical diffusion) to thermal regions and interpretation of attributes the temperature, which are outside the region of setting boundary conditions (therefore outside the size 300-400 K) at different settings of calculations factors.

The tasks were solved by using three types of grid (hexa, tetra and polyhedra). Theirs shapes were showed at Figure 2. All types of grids were had double density. Hexa and tetra cells were created from 40, or from 100 points per unit of length on all borders of region. Polyhedra's cells were created from tetra cells in software Fluent. It was begun thereby quite 6 computational regions with the same before formulated dimensions and with the number of cells showed in Table 2. It was showed there important saving of the number of cells by using polyhedra types. There important saving of the number of cells is cardinal argument for using polyhedra types in many examples, tasks.

Boundary conditions Table 1

Boundary conditions		
Entry into regions	velocity inlet	On two walls constant vertical profile was taken vector of velocity $v_x = v_y = 5$ m/s
	temperature	One wall 300 K second wall 400 K
Output out of regions	pressure outlet	$p = 0$ Pa
Side walls	symmetry	Zero's flow of all parameters trough the border and zero's normal velocity

Number of cells in computing region Table 2

Type of grid	**Hexa** 40 points	**Hexa** 100 points	**Tetra** 40 points	**Tetra** 100 points	**Polyhedra** 40 points_{tetra}	**Polyhedra** 100 points_{tetra}
Number of cells [–10^3]	12.8	200	83.9	1332	16.6	238

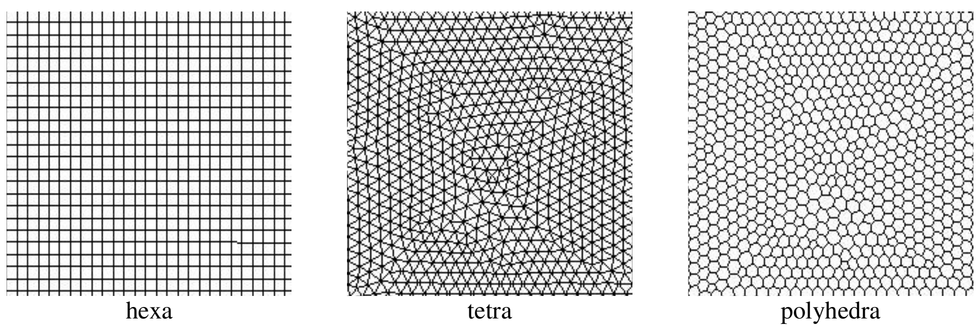


Fig. 2. *Typology of cells*

The computations with tetra and polyhedra cells were tested by using sequential setting of three computational schemas (First-order upwind, Second-order upwind, Third-order Muscl). The computation by hexa cells was done in addition by using of calculation applied the scheme Quick.

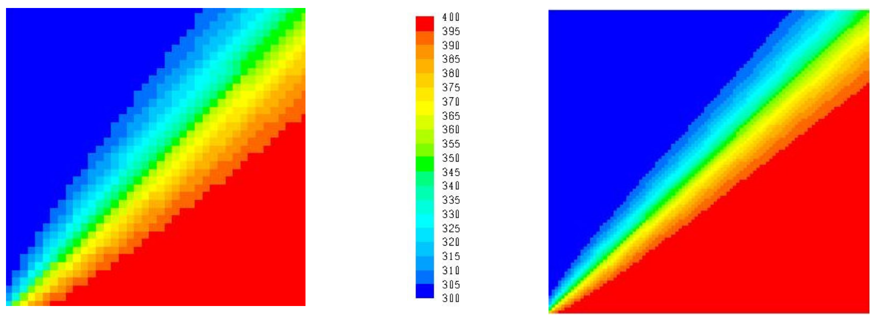
The computation of gradient by using hexa and tera cells was resolved by using Green-Gauss Cell-Based and Green-Gauss Node-Based method. It was used Green- Squares Cell-Bassed procedure at polyhedra cells, which is recommended in Fluent. All results were compared for various condition of setting of computing tasks. The computation scheme Power-law wasn't been tested, because this example was calculated equally as First-order upwind.

3. Considering of Results

The under showed images introduce temperature's field in longitudinal cuts, witch was led in the centre of computational regions by different setting of conditions of computation's schema. Scale of temperatures in Kelvin [K], (Figure 3), is valid for others pictures too. The temperature region would have been diagonal sharp divided in ideal case on two fields, there were recommended of input parameters. The temperatures wouldn't have been existed outside the amplitude 300-400 K.

3.1. Influence of density of grid

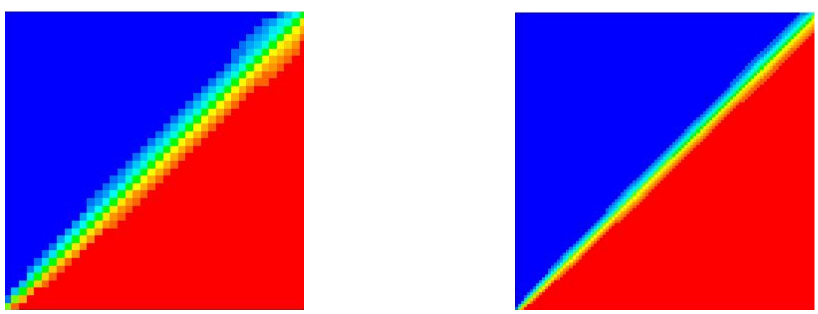
The density of grid had the major influence on the size of numerical diffusion. The thermal dispersion by hexa grid was shown on Figure 3, grid with density 40 points and 100 points per unit of length by using computational scheme First order. The density had the same influence on dispersion of thermal region by using of the others both grids. The influence of general dispersions and differences of density of grids were smaller by using of computational schemes Second-order upwind, Quick, Thirt-order Muscl (Figure 4), but there are problems with values of transportation parameter (temperature) outside amplitude of input parameters (more in Chap. 3.3).



hexa cells 40 points/m
First-order

hexa cells 100 points/m
First-order

Fig. 3. *Temperature region, influence of density of grid on numerical diffusion*



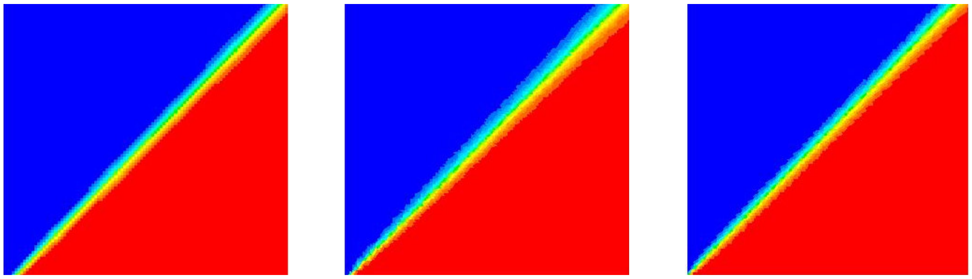
hexa cells 40 points/m
Second-order

hexa cells 100 points/m
Second-order

Fig. 4. *Temperature region, influence of density of grid on numerical diffusion*

3.2. Influence of type of grid

Typology of grid have influence at a numerically diffusion of transportation parameter too, even if not so expressive, as was seen from Figure 5. The dispersions of temperature regions were compared (in Figure 5) for all tree types of grids by comparable density (100 points per m) and by identically choosing of computing scheme (Second-order upwind). It is evident, that the smallest dispersion was achieved by using of hexa grid. It isn't possible to use this grid (hexa) due to types of computing regions and flowed solids very often. Type of grid was limited partly using of computing schema and method of computing of gradient too, it was showed on exactness of computation markedly (view next Chapter).



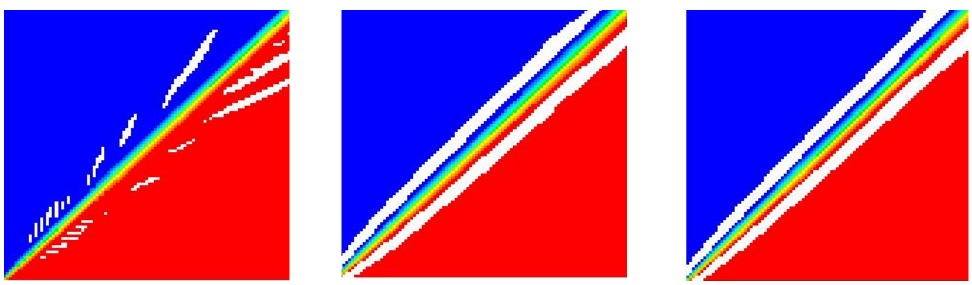
hexa 100 pt./m Second-order | tetra 100 pt./m Second-order | polyhedra 100 pt./m Second-order

Fig. 5. *Temperature region, influence of type of grid at numerical diffusion*

3.3. Influence of choose of computational schema

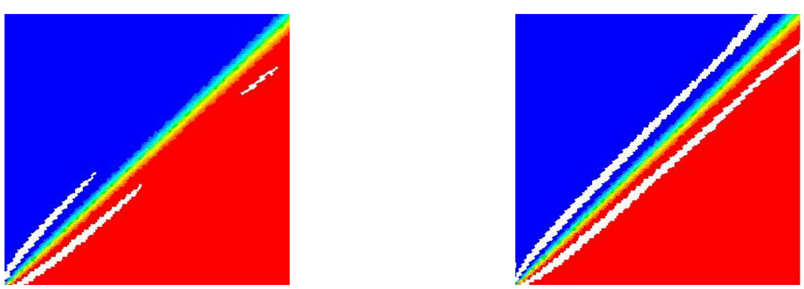
The most exact results was achieved by using Quick computing schema in the region numeric diffusion, by the smallest occurrence of values outside the region input parameters too (on Figures 6 and 7 colorless regions).

Computing schemes First-order and Power-law were showed reciprocal equivalent results. The values of temperatures weren't existed in temperature region outside the required amplitude, but the marked numerical diffusion was given by of both schemas, it was seen in Figure 3. This expressive dissipation was given for all types of grids by using these two schemes.



hexa 100 pt./m Quick | hexa 100 pt./m Second-order | hexa 100 pt./m Third-order Muscl

Fig. 6. *Temperature region, influence choosing of computational scheme on exactness of computing*



polyhedra 100 pt./m Second-order | polyhedra 100 pt./m Third-order Muscl

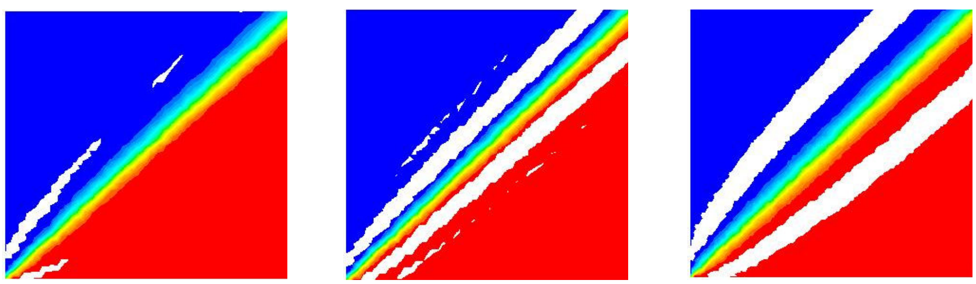
Fig. 7. *Temperature region, influence choosing of computational scheme on exactness of computing*

Tetra and polyhedra grids showed better results of computing scheme Second-order, as Third-order Muscl, it is evident from Figure 7. The lower number of cells with values outside the required region of thermal region, against hexa cells, in Figure 6 was compensated negative the higher value of divergence, as was illustrated in Chap. 3.4.

3.4. Influence of choosing computational method of solving gradient of transport parameter

Solution's method of gradient of transport parameter has decided influence at a creation of values outside the region of input parameters, as well as choice of computational's scheme. The calculations with hexa and tetra cells was solved by using of recommended Green-Gauss Cell-Based and Green-Gauss Node-Based methods, whereby better results were given by hexa by using Cell-Based method cells and better results were given by tetra cells by using Node-Based method, Figure 8.

The regions with polyhedra cells were computed by using Least Sguares Cell- bass method, which is recommended for this type cells in manual Fluent. This method achieved the worst results, mainly the highness of values of divergence from required parameters, there are seen in Figure 9. The result was compared for all variants of computing, where divergences were given.



tetra 40 pt./m Cell-Based | tetra cells 40 pt./m Node-Based | polyhedra 40 pt./m Least Sguares

Fig. 8. *Temperature region, influence choosing of computational Method of gradient transport parameter* (*computational schema Second-order*)

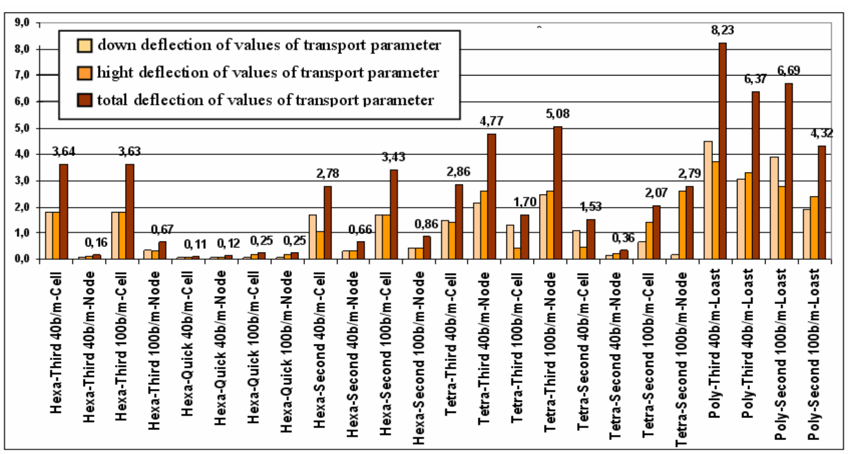


Fig. 9. *Influence of type and density of grid, computational schema and Method calculation of gradient on value temperature region outsider amplitude input parameter*

4. Conclusions

At application First-order and Power- law scheme wasn't given any temperature region outside the region of input conditions, but the large numerical diffusion reduces markedly exactness of computation.

The best results were obtained by using Hexa grid and computational scheme Quick upwind. The Method of computing of gradient has negligible influence on existence of values outside the region „good" temperature. The smaller diffusion was given by denser grid.

It is interesting knowledge's by both schema (Second-order a Third-order), that for hexa cells is explicit more accurate Node-Based Method, but for hexa cells is more accurate Cell-Based Method.

The negative knowledge's are relatively high levels values of divergence of transport parameters outside the temperature region at there necessary time of computing. The current offer possibility of calculation can't allow computation with appeased physical exactness.

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References

1. Kotrasová, K., Sojčák, D.: *Možnosť riešenia interakcie kvapaliny s nádobou pri harmonickom pohybe* (*Solution Possibility of Interaction of Fluid with Container during Harmonius Motion*). In: Civil and Environmental Engineering, Roč. 5, č. 2 (2009), s. 72-78.
2. Leoveanu, I.S., et al.: *Fluid Seismic Modelling Inside Reservoirs Walls and Shipping Channel Based on Transport Phenomena*. In: Proceedings of the 13th WSEAS International Conference on Automatic Control, Modelling & Simulation, Lanzarote, Canary Islands, Spain, 27-29 may, 2011; World Scientific and Engineering Academy and Society (WSEAS), 2011, p. 398-403.
3. Michalcová, V.: *Numerická simulace zatížení budov v reálné atmosféře při různých směrech prouzení* (*Numerical Simulation of Loading of Building in Real Atmosphere by Various Directions of Flow*). In: Zborník z konferencie „Staticko - konštrukčné a stavebno - fyzikálne problémy stavebných konštrukcií". Štrbské Pleso, Vysoké Tatry, 2006.
4. Száva, I., Kormaníková, E., Kotrasová, K.: *Reduced-Scales Models' Experimental Results Used in Further Finite Element Analysis.* In: Journal of Civil Engineering **5** (2010) Issue 3, p. 83-90.
5. Vesteeg, H.K., Malalasekera, W.: *An Introduction to Computational Fluid Dynamics*. England. Pearson Education Limited, 2007.
6. Fluent Inc. Fluent 6.3: *User's Guide.* 2003. Available at: http://sp1.vsb.cz/DOC/Fluent_6.1/html/ug//main_pre.htm. Accessed: 22-11-2011.