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PSEUDOSPECTRAL APPROXIMATION COMPARED WITH CONTROL VOLUME FORMULATION AND FINITE DIFFERENCES – SOME TEST CASES

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Abstract: The paper presents comparison of the pseudospectral method with low-order approximation for two test cases. The first test case is quasi one-dimensional supersonic flow through converging-diverging nozzle for which exact solution exists. Comparison of the error of pseudospectral approximation and upwind finite-differences using Steger-Warming flux splitting method shows high accuracy of the pseudospectral method even for few collocation points. The same conclusion is formulated for the second test case, namely incompressible flow in two-dimensional driven cavity solved by control volume formulation with modified QUICK upwinding scheme and SIMPLEC algorithm for pressure correction. As usually conclusions concerning accuracy of numerical methods are flow case dependent, but the two examples shown give some idea about the accuracy and resolution of spectral approximation versus standard CFD schemes.

Keywords: computational fluid dynamics, spectral methods, pseudospectral method, supersonic flows, driven cavity

1. Introduction

Spectral methods based on polynomial approximation of unknown function compared with classical, low-order approaches like finite elements, finite differences or control volume formulation are much more precise both in computational precision, as well as spatial resolution. For problems in which a smooth solution exists it is possible to obtain a very high accuracy with relatively few terms in spectral approximation.

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In flow problems with periodic boundary conditions in some or all direction the most often used is the Galerkin method based on the Fourier series representation of unknown function in spectral space. In the cases of flow with other types of boundary conditions high accuracy is very difficult to obtain and sometimes is not at all possible to achieve using Galerkin approach. This is for example the reason of arising instabilities connected to the oscillations near the boundaries (Gibbs phenomena). Because of various boundary condition types in the field of fluid dynamics the most often used are the pseudospectral methods. In contrast to the spectral methods for which solution is presented in terms of polynomial coefficients the solution in pseudospectral formulation is sought directly in nodal values of the unknown function.

The paper presents a comparison of pseudospectral method based on Chebyshev polynomials with low-order approximations in the following test cases:

- 2D incompressible flow in a driven cavity – comparison with control volume formulation;
- Quasi one-dimensional flow in a converging-diverging nozzle – comparison with upwind finite difference scheme using Steger-Warming flux splitting method.

For the second test case an exact solution exists which is used to evaluate the accuracy of the different approaches studied within this paper.

2. Pseudospectral approximation based on Chebyshev polynomials

The properties of the Chebyshev polynomials used widely in spectral and pseudospectral approximation are described in details in monographs of Fox and Parker [3] and Rivlin [6]. Hereafter, only the most important features allowing to approximate first- and second-order derivatives will be referred. The derivatives will be expressed only in the physical space without any transformation between physical and spectral space. For the sake of simplicity of the reasoning presented below, the pseudospectral approximation will be presented in one dimension but expansion to 2D and 3D situation is obvious.

Every dependent variable characterising the flow field can be expanded in a series of Chebyshev polynomials:

$$F(x)=\sum_{i=0}^{N}\hat{F}_i\cdot T_i(x), \tag{1}$$

where:

- $T_i(x) = \cos(i\cdot \arccos(x))$ – Chebyshev polynomial;
- $\hat{F}_i$ – coefficient of the series;
- N – number of terms in the series.

In a vector notation the approximation of the function $F(x)$ in all selected collocation points can be written collectively as:

$$\mathbf{T}\cdot\hat{\mathbf{F}}=\mathbf{F}. \tag{2}$$

Using the Chebyshev-Gauss-Labatto [1] collocation points defined as:

$$x_k = \cos\left(\frac{\pi \cdot k}{N}\right), \tag{3}$$

the first and second derivatives of a function $F(x)$ in vector notation can be written as:

$$\frac{\partial \mathbf{F}}{\partial x} = \hat{\mathbf{G}}^{(1)} \cdot \mathbf{F}, \qquad \hat{\mathbf{G}}^{(1)} = \mathbf{T} \cdot \mathbf{G}^{(1)} \cdot \mathbf{T}^{-1}, \tag{4}$$

$$\frac{\partial^2 \mathbf{F}}{\partial x^2} = \hat{\mathbf{G}}^{(2)} \cdot \mathbf{F}, \qquad \hat{\mathbf{G}}^{(2)} = \mathbf{T} \cdot \mathbf{G}^{(2)} \cdot \mathbf{T}^{-1}, \tag{5}$$

where the coefficients of matrices $\mathbf{G}^{(1)}$, $\mathbf{G}^{(2)}$, $\mathbf{T}^{-1}$ are given by the following relations:

$$\begin{aligned} G^{(1)}_{j,m} &= 0 \qquad \text{for} \quad j \geq m \ \text{or} \ j = m \ \text{even}, \\ G^{(1)}_{j,m} &= 2 \cdot m / c_k \qquad \text{otherwise}, \end{aligned} \tag{6}$$

where:

$$\begin{aligned} c_k &= 2 \quad \text{for} \quad j = 0, \\ c_k &= 1 \quad \text{for} \quad j > 0; \end{aligned}$$

$$\mathbf{G}^{(2)} = \mathbf{G}^{(1)} \cdot \mathbf{G}^{(1)}; \tag{7}$$

$$T^{-1}_{j,k} = \frac{2}{N} \cdot \frac{1}{c_j} \cdot \frac{1}{c_k} \cdot T_j(x_k), \tag{8}$$

where:

$$\begin{aligned} c_j = c_k &= 2 \quad \text{for} \quad j,k = 0 \ \text{or} \ N, \\ c_j = c_k &= 1 \quad \text{for} \quad 0 < j, \ k < N. \end{aligned}$$

There are of course other possibilities [1] to calculate derivatives by using the Fast Fourier Transform between spectral and physical space but for the calculations performed with a relatively small number of the collocation points ($N < 32$) the method presented above is satisfactory.

3. Solution of quasi one-dimensional compressible inviscid flow

3.1 Pseudospectral approximation of 1D Euler's equations

As the first test case, we consider a quasi one-dimensional compressible inviscid flow through the converging-diverging nozzle of a given shape $S(x)$. The governing continuity, momentum and energy equations for this problem [4] in conservative form can be written as follows:

$$\frac{\partial \mathbf{U}}{\partial t}+\frac{\partial \mathbf{Q}}{\partial x}=\mathbf{H}, \tag{9}$$

where:

$$\mathbf{U}=\begin{vmatrix}\rho\\ \rho\cdot u\\ \rho\cdot u\cdot E\end{vmatrix},\quad \mathbf{Q}=\begin{vmatrix}\rho\cdot u\\ \rho\cdot u^2+p\\ \rho\cdot u\cdot(E+p/\rho)\end{vmatrix}, \tag{10}$$

$$\mathbf{H}=\begin{vmatrix}-\rho\cdot u\cdot S/S'\\ -\rho\cdot u^2\cdot S/S'\\ -(\rho\cdot u\cdot E+u\cdot p)\cdot S/S'\end{vmatrix} \tag{11}$$

with equation of state:

$$p=(\gamma-1)\cdot\rho\cdot(E-u^2/2), \tag{12}$$

and given shape $S(x)$ of the nozzle:

$$S(x)=0.1+0.5\cdot(0.1+0.5\cdot x)^2,\qquad S'(x)=\frac{dS(x)}{dx}. \tag{13}$$

The analytical solution to this problem as well as relations between Mach number and pressure, temperature, *etc.* can be found in many sources and will not be given here.

Applying the rule (presented in the preceding section) of the approximation of the first derivative to each of the equations (9) leads to the following semi-discrete form:

$$\frac{\partial \mathbf{U}_k}{\partial t}+\hat{\mathbf{G}}^{(1)}\cdot\mathbf{Q}_k=\mathbf{H}_k,\qquad k=1,2,3, \tag{14}$$

where for instance for $k=1$ vectors $\partial \mathbf{U}_1/\partial t$, $\mathbf{Q}_1$ and $\mathbf{H}_1$ represent values in the selected collocations points of vectors (10) and (11) corresponding to their first elements as follows:

$$\frac{\partial \mathbf{U}_1}{\partial t}=\frac{\partial}{\partial t}\begin{vmatrix}\rho|_{x_0}\\ \rho|_{x_1}\\ \cdots\\ \cdots\\ \rho|_{x_N}\end{vmatrix},\quad \mathbf{Q}_1=\begin{vmatrix}(\rho\cdot u)|_{x_0}\\ (\rho\cdot u)|_{x_1}\\ \cdots\\ \cdots\\ (\rho\cdot u)|_{x_N}\end{vmatrix},\quad \mathbf{H}_1=\begin{vmatrix}(-\rho\cdot u\cdot S/S')|_{x_0}\\ (-\rho\cdot u\cdot S/S')|_{x_1}\\ \cdots\\ \cdots\\ (-\rho\cdot u\cdot S/S')|_{x_N}\end{vmatrix}. \tag{15}$$

3.2 Results of computations

In order to compare the spatial accuracy of the Chebyshev collocation pseudospectral method, equations (9) were additionally solved by one of the standard methods used for this type of flow problems, namely upwind difference

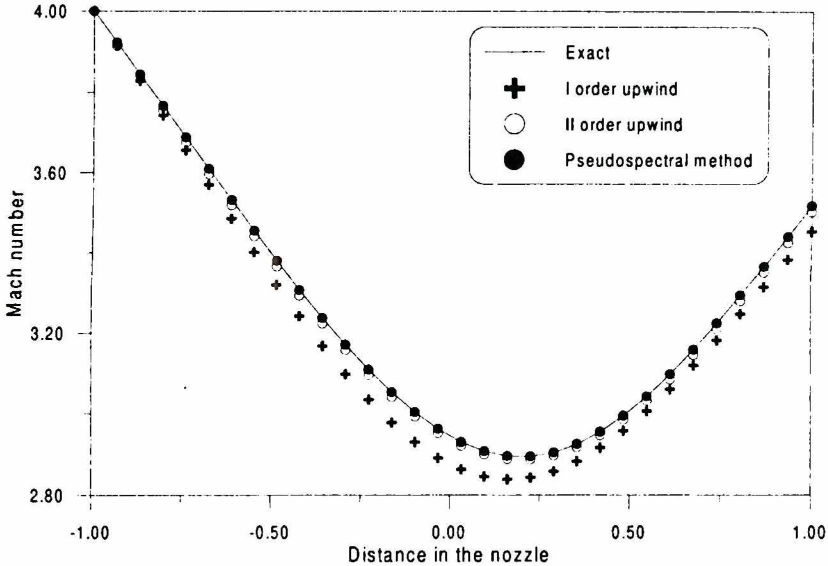

***Figure 1.** Distribution of the Mach number along the nozzle*

scheme in connection with the Steger-Warming flux splitting method [7]. In both cases discretization in time was performed using second order predictor-corrector method, where first-order Adams-Bashforth scheme was used as a predictor and the second-order Adams-Multon algorithm as a corrector. Figure 1 presents the distribution of the Mach number along the nozzle for supersonic case, where the inlet Mach number was Ma = 4.0, whereas two remaining inlet boundary values were obtained from the thermodynamic relations with imposed reference (stagnation) values $p = 0.5$ MPa and $T = 500$ K.

The results presented were obtained for 16 collocation points in the case of pseudospectral method and for 32 nodes for upwind difference scheme. The collocation points applied in pseudospectral method are not uniformly spaced and the results shown in Figure 1 were obtained by interpolation. It is clearly seen from Figure 1 that the first-order upwind difference scheme is completely unsatisfactory (as was expected), whereas accuracy of the second-order upwind difference scheme is significantly better but in comparison to the results obtained using the pseudospectral method it is still much worse. To show the differences between analytical and numerical solution, we defined the following measure of the error:

$$\varepsilon = \sum_{i=1}^{N} \frac{\left| F_i^{exact} - F_i^{num} \right|}{N}. \tag{16}$$

The error defined by (16) for different numerical methods and different mesh sizes is compared in Table 1. It should be noted that the error presented for the pseudospectral method is additionally biased by an error arising from the interpolation used to obtain dependent variables in the uniformly spaced nodes which correspond to equally spaced mesh points used in upwind difference calculations.

It can be seen from the results presented in Table 1 that the pseudospectral method with 16 collocation points gives an order of magnitude more accurate solution than the second order upwind finite difference scheme. Moreover, doubling the number of the collocation points gives three orders of magnitude more accurate solution, while in the case of low-order scheme only one order of magnitude decrease of the error is observed.

Table 1. *Difference between an exact and numerical solution*

	Pseudospectral metod		*Second-order upwind difference*	
	16 points	24 points	50 points	100 points
Mach number	2.2 e-4	4.7 e-7	4.5 e-3	1.1 e-3
Temperature	1.4 e-2	3.2 e-5	3.0 e-1	7.5 e-2
Pressure	1.4 e+0	3.0 e-3	3.0 e+1	7.9 e+0

4. Solution of 2D incompressible flow

4.1 Pseudospectral approximation of Navier-Stokes equations

As a second test case the unsteady flow in a driven cavity was chosen, for which the non-dimensional form of Navier-Stokes equations are given by:

$$\frac{\partial u}{\partial t}+\frac{\partial (u\cdot u)}{\partial x}+\frac{\partial (u\cdot v)}{\partial y}=-\frac{\partial p}{\partial x}+\frac{1}{\mathrm{Re}}\cdot\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right), \tag{17}$$

$$\frac{\partial v}{\partial t}+\frac{\partial (u\cdot v)}{\partial x}+\frac{\partial (v\cdot v)}{\partial y}=-\frac{\partial p}{\partial y}+\frac{1}{\mathrm{Re}}\cdot\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right). \tag{18}$$

According to the rules presented in Chapter 2 the partial derivatives appearing in Navier-Stokes equations can be presented as follows:

$$\left.\frac{\partial (u\cdot u)}{\partial x}\right|_{j,k}=\sum_{m=0}^{N_x}\hat{G}^{x(1)}_{j,m}\cdot (u\cdot u)\Big|_{m,k},$$

$$\left.\frac{\partial (u\cdot v)}{\partial y}\right|_{j,k}=\sum_{m=0}^{N_y}\hat{G}^{y(1)}_{k,m}\cdot (u\cdot v)\Big|_{j,m},$$

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{j,k}=\sum_{m=0}^{N_x}\hat{G}^{x(2)}_{j,m}\cdot u\Big|_{m,k}, \tag{19}$$

$$\left.\frac{\partial^2 u}{\partial y^2}\right|_{j,k} = \sum_{m=0}^{N_y} \hat{G}^{y(2)}_{k,m} \cdot u\Big|_{j,m},$$

where $\hat{G}^{x(1)}_{j,m}$, $\hat{G}^{y(1)}_{k,m}$, $\hat{G}^{x(2)}_{j,m}$ and $\hat{G}^{y(2)}_{k,m}$ are the coefficients of matrices $\hat{\mathbf{G}}^{(1)}$ and $\hat{\mathbf{G}}^{(2)}$ given in the preceding section.

The Navier-Stokes equations completed by the continuity equation were solved by the projection method [2] that allows in an explicit way to determine the pressure field in a new time step by the use of the continuity equation. It should be noted that the Poisson equation for pressure arising in the projection method was approximated in the same manner as the Navier-Stokes equations.

4.2 Results of computations

In order to compare the pseudospectral method with a low-order scheme, like in the previous test case, the flow problem was solved by finite volume method using modified QUICK (Quadratic Upwind Interpolation for Convection Kinematics) scheme [5] to approximate the convection terms in the Navier-Stokes equations and SIMPLEC algorithm to determine pressure field.

The calculations were performed for Reynolds number defined by the velocity of the upper wall and the cavity depth Re = 1000. The results obtained by both numerical approaches were shown for control cross-sections located at $x/H = 0.2$, 0.4, 0.6, 0.8. Grid-independence for the pseudospectral method was obtained for the mesh of 26×26 collocation points in each direction. Figures 2-4 show results obtained by pseudospectral method and control volume formulation for the meshes 30×30, 60×60 and 80×80. The results presented refer to steady state solution.

From the results presented it is clearly seen that the grid-independent solution is obtained by pseudospectral with much coarser grid than in the case of low-order control volume formulation. Table 2 shows the error defined with analogy to equation (16), where instead of the exact solution the results of the pseudospectral method were used.

Table 2. *Error of the u-component velocity approximation*

Number of finite volumes	*Cross-section x/H*			
	0.2	0.4	0.6	0.8
30×30	0.076	0.083	0.064	0.092
60×60	0.034	0.026	0.019	0.041
80×80	0.0015	0.001	0.001	0.0014

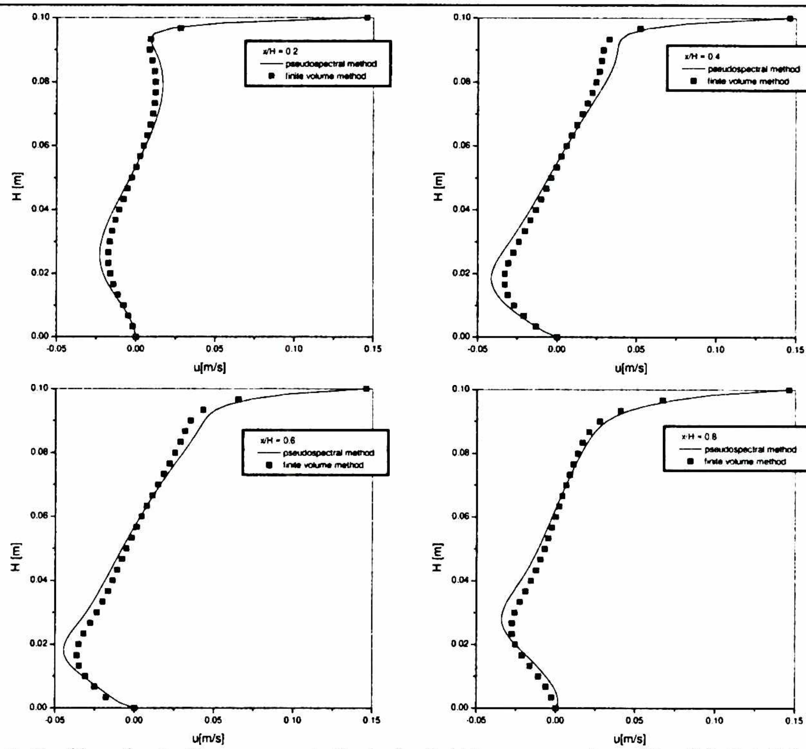

Figure 2. *Profiles of u [m/s] component of velocity field in cross-section x/H = 0.2, 0.4, 0.6, 0.8 obtained at 30×30 control volumes*

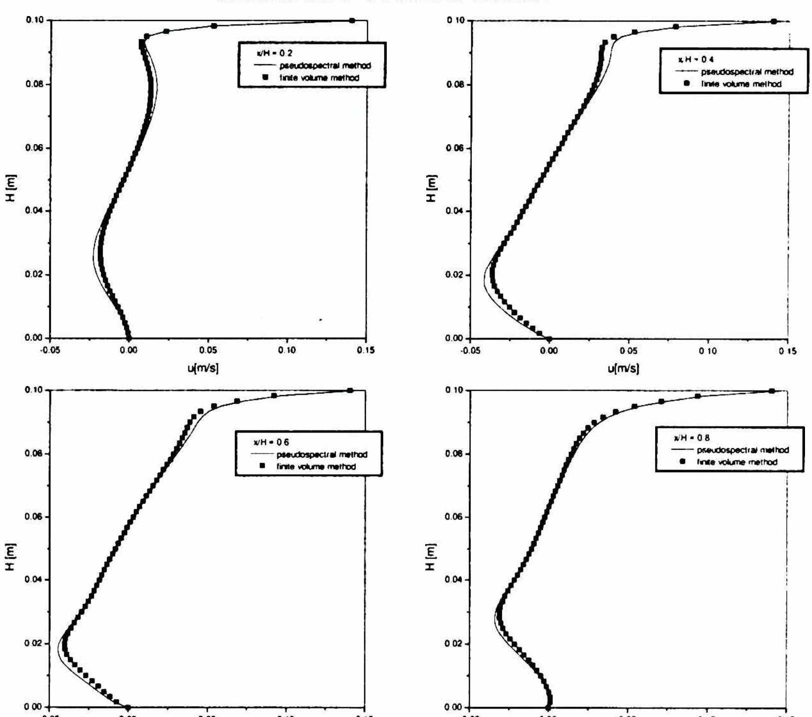

Figure 3. *Profiles of u [m/s] component of velocity field in cross-section x/H = 0.2, 0.4, 0.6, 0.8 obtained at 60×60 control volumes*

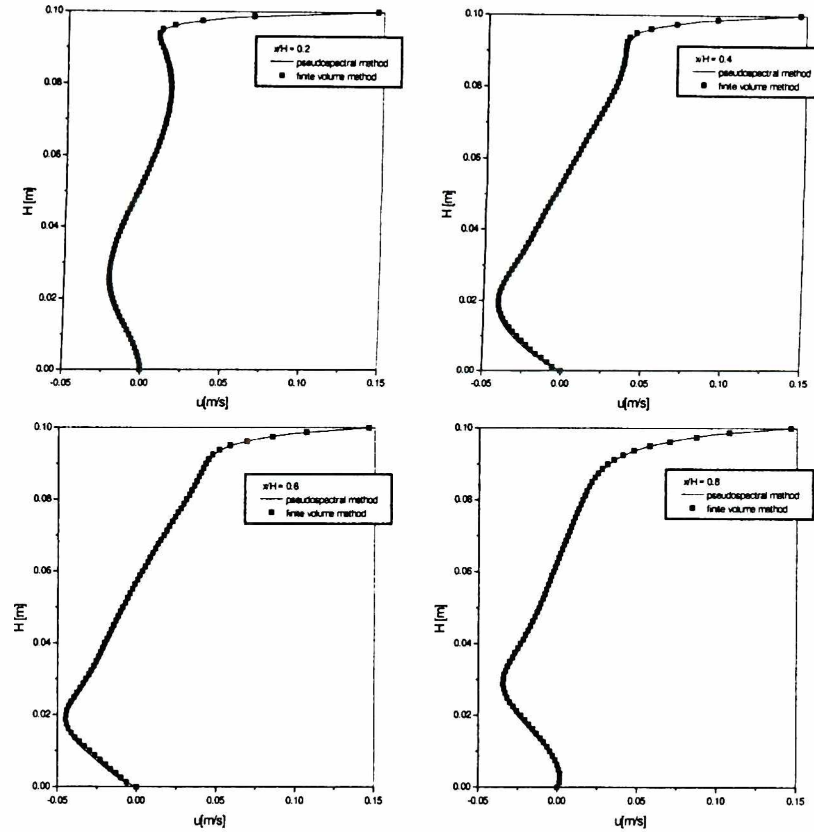

Figure 4. *Profiles of* u *[m/s] component of velocity field in cross-section x/H = 0.2, 0.4, 0.6, 0.8 obtained at 80×80 control volumes*

5. Concluding remarks

The paper presents the results of numerical predictions in two relatively simple test cases. These flow problems were utilised to compare the efficiency and spatial resolution of the pseudospectral method based on Chebyshev polynomial series with classical methods used in CFD. In both cases studied in the paper, namely the one-dimensional compressible flow and two-dimensional incompressible problem of the driven cavity very high numerical accuracy of the pseudospectral method was confirmed. It should be underlined here that the computational efficiency of the pseudospectral method is possible because of very rapid decrease of the approximation error with the number of terms in spectral expansion.

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