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High-Order Methods for the Numerical Simulation of Vortical and Turbulent Flows

A multigrid pseudo-spectral method for incompressible Navier–Stokes flows

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Abstract

A pseudo-spectral solver with multigrid acceleration for the numerical prediction of incompressible non-isothermal flows is presented. The spatial discretization is based on a Chebyshev collocation method on Gauss–Lobatto points and for the discretization in time the second-order backward differencing scheme (BDF2) is employed. The multigrid method is invoked at the level of algebraic system solving within a pressure-correction method. The approach combines the high accuracy of spectral methods with efficient solver properties of multigrid methods. The capabilities of the proposed scheme are illustrated by a buoyancy driven cavity flow as a standard benchmark case. ***To cite this article: K. Krastev, M. Schäfer, C. R. Mecanique 333 (2005).***

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1. Introduction

Despite the advances in computational fluid dynamics in recent years, the reliable numerical simulation of complex transient three-dimensional flows must still be considered as a challenge with respect to computational resources. Therefore, the further improvement of corresponding numerical techniques is an issue of high practical interest.

With respect to discretization, the outstanding properties of spectral methods with their high order of accuracy are well known. Having their roots in the fourth decade of the previous century, spectral methods have been intensively developed and studied the last 30 years. Starting from the pioneering theoretical monograph of Gottlieb and Orzag [1], there are a variety of other works documenting and analysing the directions and scientific achievements in the field (e.g. [2–5]).

Among the solution techniques for the algebraic systems resulting from a discretization scheme, multigrid techniques have proven to yield a significant improvement in computational performance. The basics of multigrid

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methods are described, for instance, in [6] or [7]. Typically, multigrid techniques are applied in connection with finite-volume or finite-element methods (e.g. [8,9]), i.e. in the context of *sparse* algebraic system solving.

The present work tries to combine the advantages of spectral discretizations and multigrid solvers. The underlying spectral approach consists in the Chebyshev pseudo-spectral method presented in details in [10,11]. The involvement of a multigrid procedure aims to further increase the computational efficiency of this scheme. The multigrid method is used as a solver for the various *dense* algebraic systems resulting from the spectral discretization in the course of a pressure-correction method. To the authors best knowledge the coupling of Chebyshev pseudo-spectral and multigrid methods has not been reported so far in the literature.

For simplicity, we only consider here incompressible flows governed by the Boussinesq approximation within orthogonal mono-block domains. Possible extensions to more general situations with respect to physical and geometrical complexity are discussed in [11].

2. Governing equations

We consider the non-isothermal flow of an incompressible Newtonian fluid. The corresponding balance equations for mass, momentum, and energy can be written in the following non-conservative form:

$$\frac{\partial u_j}{\partial x_j} = 0 \tag{1}$$

$$\rho \frac{\partial u_i}{\partial t} - \mu \frac{\partial^2 u_i}{\partial x_j^2} + \rho u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \rho_{\mathrm{R}} \beta (T - T_{\mathrm{R}}) g_i \tag{2}$$

$$\rho c_p \frac{\partial T}{\partial t} - \lambda \frac{\partial^2 T}{\partial x_j^2} + \rho c_p u_j \frac{\partial T}{\partial x_j} = \rho f \tag{3}$$

where u_i represents the velocity component with respect to Cartesian coordinates x_i, t is the time, p is the pressure, ρ is the fluid density, μ is the dynamic viscosity, g_i is the gravitational acceleration vector, T is the temperature, c_p is the heat capacity coefficient at constant pressure, λ is the heat diffusion coefficient, and f are volume heat sources. For taking into account the temperature influence on the density field the Boussinesq approximation is used, i.e. the density is assumed to be (linearly) dependent on the temperature only in the volume force term of the momentum equations (2). ρ_{R} and T_{R} are corresponding reference values for the density and temperature, respectively, and β denotes the volumetric expansion coefficient. All other material properties are assumed to be constant in space and time. The equation system (1)–(3) has to be completed by suitable boundary and initial conditions for u_i and T.

Following the similarities in the structures of Eqs. (2) and (3) we define the generalized scalar transport equation

$$\tilde{\rho} \frac{\partial \phi}{\partial t} - \Gamma \frac{\partial^2 \phi}{\partial x_j^2} + \Lambda^j \frac{\partial \phi}{\partial x_j} = F \tag{4}$$

for which, for ease of presentation, all following numerical techniques will be described. The quantities $\tilde{\rho}$, Γ, Λ^j, and F represent the respective coefficients and source terms in Eqs. (2) and (3).

3. Discretization scheme

We assume orthogonal problem domains which can be mapped to the unit cube with a simple stretching in each of the spatial directions. Regarding the discretization procedure, we closely follow techniques described in [3]. A brief summary is given in the following. Chebyshev-collocation method on the Gauss–Lobatto points.

The time derivative is approximated by the second order backward Euler scheme and of the non-linear term in the momentum conservation equations (2) is evaluated by a second-order Adams–Bashfort extrapolation

$$\Lambda^j\big|_{t=t_n} \approx 2\Lambda^j\big|_{t=t_{n-1}} - \Lambda^j\big|_{t=t_{n-2}} \tag{5}$$

giving the scheme a semi-implicit character.

Due to the separation of the spatial variables, the discrete approximation of the derivatives in each direction is determined only with the help of the discrete function values on the grid line coinciding with the concrete spatial direction in a finite-difference-like manner [12].

Denoting by $D^k_{i_k\alpha}$ the discrete differential operator in the spatial direction x_k, the final discrete linear system for the general scalar transport equation for each time step can be written as:

$$\frac{3\tilde{\rho}}{2\Delta t}\phi^n_{i_1i_2i_3} + \sum_{\gamma=1}^{3}\left[-\Gamma_{i_1i_2i_3}(D^\gamma_{i_\gamma\alpha})^2 + \Lambda^\gamma_{i_1i_2i_3}D^\gamma_{i_\gamma\alpha}\right][\delta_{\alpha i_\gamma}\phi^n_{i_1i_2i_3}] = \widetilde{F}^n_{i_1i_2i_3} \tag{6}$$

at all internal nodal points at time level $t = t_n$. $\widetilde{F}^n_{i_1i_2i_3}$ contains the discrete representation of the external sources as well as the terms arising from the time discretization and the boundary conditions treatment while Λ^j is determined from (5). Remark that Einstein summing is performed over the silent index α and the Kroneker symbol is used to determine the position of the running index in $\phi_{i_1i_2i_3}$ with respect to the spatial direction part of the discrete derivative operator.

4. Pressure-correction scheme

The coupling of the primitive variables is solved using a pressure-correction scheme similar to those proposed by Gresho [13] and van Kan [14], which have been investigated in detail by Turek [15]. A detailed description of the scheme can be found in [11]. So, we just summarize the basic ideas here.

First, using the values of the pressure at the previous time step p^{n-1}, a predicted velocity field $\tilde{u}^n_i$ which is not divergence free, is computed from the discrete momentum equations. To fulfil the discrete continuity equation a Poisson equation

$$\frac{\partial^2 q^n}{\partial x_j^2} = \frac{\partial \tilde{u}^n_j}{\partial x_j} \tag{7}$$

with homogenous Neumann boundary conditions is solved for the pressure-correction q^n, which is than used to correct the velocity and the pressure fields:

$$p^n = p^{n-1} + \alpha_R\frac{3\rho}{2\Delta t}q^n - \alpha_D\mu\frac{\partial \tilde{u}^n_j}{\partial x_j} \tag{8}$$

$$u^n_i = \tilde{u}^n_i - \frac{\partial q^n}{\partial x_i} \tag{9}$$

The two parameters α_R and α_D can be used to control the convergence of the scheme (see [15]). In our numerical example in Section 6 the values $\alpha_R = 0.1$ and $\alpha_D = 1$ are used. Finally, the time step is completed by solving the discrete energy equation to obtain the temperature T^n.

5. Multigrid solver

The above pressure-correction scheme requires the solution of various linear systems for the velocity components, the pressure correction, and the temperature within each time step. In [11] these linear systems are solved with restarted GMRES solver. Here, we propose the use of a multigrid technique, which proved to be very efficient within the context of finite-volume or finite-element schemes (e.g. [8]).

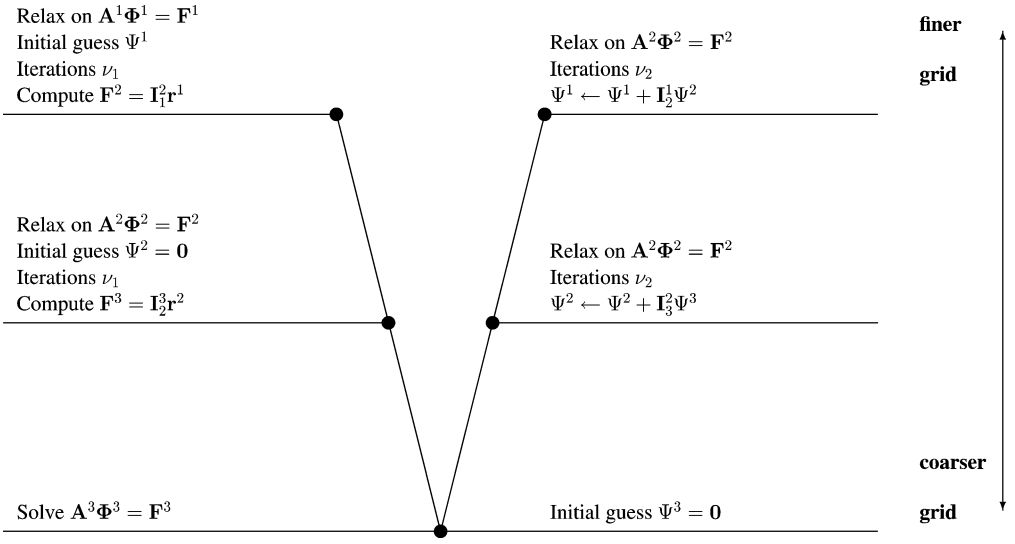

Fig. 1. Schematic view of multigrid V-cycle.

For the basic concepts of multigrid methods we refer to [6]. The key idea is to transfer the residual of the system to a coarser grid, where a faster reduction of the low frequency error modes is possible. For the movement through the grid levels we employ a classical V-cycle approach, which is illustrated schematically in Fig. 1. Here, the linear system on grid level i is denoted by

$$\mathbf{A}^i \boldsymbol{\Phi}^i = \mathbf{F}^i \tag{10}$$

$\mathbf{r}^i$ is the corresponding residual, and $\mathbf{I}_j^i$ are the transfer operators from grid level i to j (restriction and prolongation). The values of the two parameters ν_1 and ν_2 define the number of pre- and post-smoothing steps.

The linear systems on the different grid levels are obtained by applying the pseudo-spectral scheme as described above on the corresponding grids. The formation of the system matrices in (10) is made using the representation (6) together with the linearization technique (5) and a boundary conditions in the following way:

The discrete differential operators are determined on each of the grid levels, as a preprocesing step. On the top level (finnest) grid the computed quantities have their boundary conditions directly determined from the physical problem and the applied numerical techniques. The boundary conditions on the lower grid levels transfered as type to the corresponding projections in homogeneous manner. The computed linearization of Λ^j is transfered between the grid levels using the restriction operators $\mathbf{I}_j^i$ from the initially computed value on the finnest grid.

As smoothing iteration the restarted GMRES method with a one-dimensional Krylov subspace (e.g. [16]) is employed. On the coarsest grid, the smoother is used as a solver until a given convergence criterion is reached.

For the intergrid transfers of the residuals, the residual computed on the grid is interpolated on the other one by using a Chebyshev interpolation. Due to the fact that the coarser grid points are subsets of the finer grid points the restriction from a finer to a coarser grid can be simplified by using directly the values of the points that collocate for the corresponding grids.

6. Numerical example

The implemented pseudo-spectral multigrid scheme is tested on the buoyancy driven flow in a square cavity which is a well known benchmark case (see e.g. [17]). The problem parameters are chosen to result in a Prandtl number of $Pr = 0.71$ and a Rayleigh number of $Ra = 10^5$. The setup of the problem and the resulting temperature

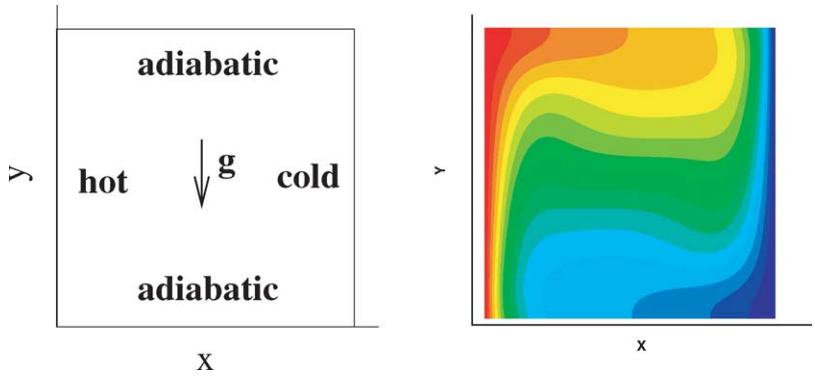

Fig. 2. Buoyancy-driven flow in a square cavity, $Pr = 0.71$, $Ra = 10^5$. Problem configuration (left) and isolines of the temperature field (right).

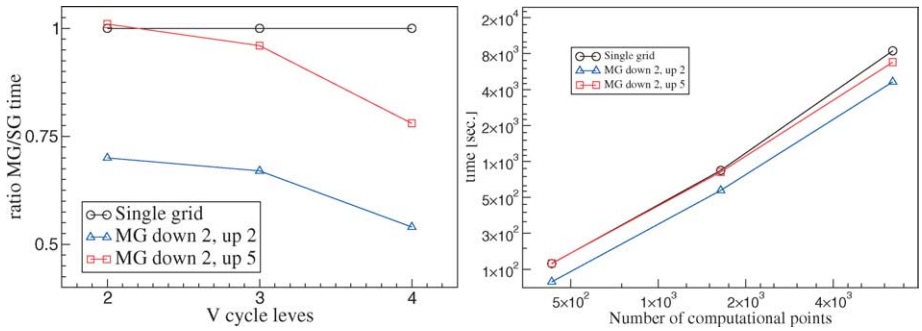

Fig. 3. Comparison of CPU times for multigrid and single grid computations (Compaq AlphaServer ES40 677 MHz).

distribution are shown in Fig. 2. As criterion to measure the performance of the schemes the computing times for reaching a fixed error value of the Nusselt number $Nu = 4.52163$ are considered.

We consider four grid levels, starting from the coarsest grid with 11×11 grid points to the finest grid with 81×81 grid points.

In Fig. 3 the absolute and relative CPU times for the multigrid scheme compared to the CPU times for the corresponding single grid scheme are shown for two choices of the parameters ν_1 and ν_2. The acceleration achieved with the multigrid scheme clearly shows. As is typical, the multigrid superiority increases with the grid size and the number of grid levels within the V-cycle.

The presented Multigrid technique does not claim to be the most efficient approach for the considered computational case. The diagonalization procedure proposed in [18] is the most efficient technique in the case of explicit convective terms; hence it is direct. The proposed semi-implicit discretization of the equations can be solved very efficiently by a preconditioned restarted GMRES iteration with a sensitively bigger dimension of the Krilov subspace and a preconditioner based on mentioned above direct Helmholtz solver, as shown in [11]. The results of those two approaches and the presented one in sense of efficiency are not comparable. The parameters for the smoother are chosen in a way that results in bigger iteration numbers and allows testing of the Multigrid scheme. However, the direction where the proposed technique could gain a real improvement of performance is in cases of Multi-domain problems, turbulence models and non-constant material properties equations, where the structure of the resulting from the pseudo-spectral discretization linear system becomes more complex and a direct procedure could not be applied. A combination of those techniques with the present Multi-grid approach needs a very good planning of the code design. The concept of integration has to be specified at the beginning of the realization and often the absence of a such a concept could be the major problem for the extension of the pseudo-spectral methods.

7. Conclusion

A pseudo-spectral multigrid method has been presented that attempts to combine the features of spectral discretization accuracy and efficient algebraic system solution. It has been shown that the use of the implemented multigrid V-cycle scheme increases the computational performance of pseudo-spectral methods for non-isothermal incompressible flows. The ratio between the CPU times for single grid and multigrid computations increases with the refinement of the grid and the number of the grid levels.

In summary, the results show that multigrid ideas can also help to improve computations based on spectral discretizations involving dense algebraic systems. Although, the multigrid acceleration is less than in the framework of finite-volume or finite-element discretizations involving sparse algebraic systems, the improvements can help to further enlarge the capabilities of spectral methods for complex flow problems.

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