NONUNIFORM PADÉ BASED COMPACT SCHEMES FOR FLUID AND HEAT FLOW PROBLEMS: DEVELOPMENT AND APPLICATION

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BY
DHARMARAJ DEKA
Roll No. MSP17104
(Reg. No. TZ156117)

DEPARTMENT OF MATHEMATICAL SCIENCES
TEZPUR UNIVERSITY, NAPAAM 784028, ASSAM, INDIA
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Chapter 6

Concluding remarks and future scopes

6.1 Observations and remarks

The work pertains to the development of finite difference based compact schemes for both 2D and 3D CDE in general and incompressible viscous flows in particular. To start with, a new class of compact schemes are developed on nonuniform cartesian grids that does not encourage any domain transformation. Subsequently, it was found that the extension of this scheme to the polar coordinate system is rather straightforward. Being developed on nonuniform meshes, the schemes are less computation expensive as there is a leverage of accumulating more grid points in regions with higher gradients and otherwise. In contrast to the earlier compact schemes, the present method is able to approximate compactly the second-order mixed derivative terms appearing in the generalized convection-diffusion type of equations with second-order convergence. The schemes are first employed on problems with analytical solutions followed by some physical problems involving mass as well as heat transfer with varying complexities to check their accuracy and robustness. Comprehensive validation study is performed by comparing the present numerical solutions with established numerical, experimental and analytical results. The work helps understand critical flow phenomenon.

Highlights of the thesis are as follows:

- A versatile compact finite difference scheme for the generalized 3D steady CDE is developed, which is, to the best of the authors knowledge, the first attempt to compactly approximate 3D generalized CDE on nonuniform grids without using any transformation. To find the solution at any point, the scheme requires at most 19 neighbouring grid points, in contrast to the previously available schemes which are based on 27 points. The scheme is employed to various linear and nonlinear PDEs and it is seen to be very efficient in all the cases. Special attention is given on the equations whose solutions possess sharp boundary layers which reveals the ability of the scheme in dealing with extreme grid clustering. To test our scheme, we mainly envision two grids: one generated geometrically and the other trigonometrically. To our satisfaction, the present scheme performed well for both type of nonuniformity. Though the present scheme has theoretical accuracy of second-order, the order of convergence was observed to approach the highest attainable order four in each cases. The accuracy of the scheme can be ascertained from the computed results which are in excellent agreement with the analytical and numerical results from some of the well established studies from the literature.

- Next, we proposed a compact, implicit finite difference scheme for 2D transient CDE for rectangular coordinate system. Theoretically, the formulation is found to be second-order accurate in both space and time. We first apply the scheme to linear problems with analytical solutions. For these problems, the scheme shows a spatial accuracy of order four. Then the scheme is employed to flow problems of different complexities, which includes the classical problems like lid-driven cavity and flow past a square cylinder. The flow problems governed by both primitive variable and streamfunction-vorticity form of the N-S equations are being considered to investigate the adaptability of the scheme. Additionally, to deal with the Neumann boundary conditions, we have introduced one-sided approximations for first-order spatial derivatives. Accurate capturing of periodic flows near and beyond the important Hopf bifurcation points for both internal and external fluid body interaction problems highlights the robustness of the scheme. We further explored the diversity of our scheme by elegantly resolving all the characteristics of heat transfer in a thermally-driven square cavity governed by the Boussinesq equations. A wide range of parameters are considered for simulation of the test problems. The computed results are compared with existing benchmark solutions and they are found to exhibit extreme proximity with each other. In majority of the cases, the present scheme could report more accurate solutions in comparison to the other studies, despite using significantly lesser grid points. Numerical convergence of the scheme has also been tested. For problems without analytical solutions, we have reported what is known as the perceived order of convergence. Additionally, to provide a insight of computational cost, the relative CPU time is also been presented wherever necessary.

- The compact scheme for 2D transient CDE on Cartesian coordinates mentioned above is extended to nonuniform cylindrical polar coordinates to investigate heat transfer and fluid flow around bluff bodies. Besides, a novel third-order accurate HOC scheme is also developed. In contrast to the most of compact schemes developed in polar coordinates, as available in the literature, there is no necessity to transform domain for the present scheme. A comprehensive comparison between the second-order accurate and third-order accurate schemes is also carried out. We begin the study by employing our scheme to two test problems having analytical solutions, followed by time marching simulation for driven polar cavity and natural convection in horizontal concentric annulus. In the process, a one-sided approximation for the vorticity boundary condition of Neumann type is also developed. The scheme is found to be well capable of handling complex flow patterns as it combines the advantages of body fitted mesh as well as nonuniformity of grids. The scheme reported a second-order temporal convergence and in space it approached to fourth-order convergence for problems with analytical solutions. For the cases where no analytical solutions are available, we have determined the perceived rate of convergence in space, and it was found to be of order three for all the variables. The computed values of various flow parameters are being compared to the values available in the literature. Results carry significant closeness to the available experimental and numerical results in all the cases, in both qualitative and quantitative sense.

- Finally, we proceed to perform a detailed numerical investigation of flow past a circular cylinder using the transient scheme mentioned above. The scheme could resolve all the trademark characteristics associated with the flow for Re values ranging from 10 to 9500. For moderate and low Re values, the flow is simulated until a steady or periodic state is reached, whereas we compute the flow in the very early span for the higher values of Re. Accurate capture of the flow in all the subranges of Reynolds numbers under consideration, such as the steady flow for $10 \leq Re \leq 40$, long time periodic flow for $100 \leq Re \leq 300$, secondary phenomena for moderate Re ($300 \leq Re \leq 1000$) and the α- and β-phenomena for higher ones ($3000 \leq Re \leq 9500$), highlights the effectiveness and robustness of the scheme. The streaklines that are produced by time integrating the paths of several weightless particles released upstream of the cylinder and time history of C_D and C_L are used to further analysis the vortex shedding process. We carry out a comprehensive comparison of our results with the experimental and other numerical results available in literature. Excellent match can be seen in all the cases both qualitative and quantitative sense.

6.2 Challenges faced

One of the main challenges associated with implementing compact schemes is solving the corresponding algebraic system of equations. For an efficient solution, it is imperative to adopt a stable solver. In this context, we have endeavoured to use modern iterative solvers. In this work, we have implemented the Krylov subspace-based solver Bi-Conjugate Gradient Stabilized (BiCGstab) without preconditioning. A discrete system solved using BiCGStab is seen to provide additional strength while efficiently simulating complex flow problems.

Another typical challenge associated with Padé-based schemes is the estimation of flow gradients at the boundaries. In this study, we have adopted a problem-specific approach. Thus, physical conditions wherever available, have been incorporated, and in their absence, flow gradients have been estimated numerically at the boundaries.

6.3 Shortcomings

A typical limitation of schemes developed for nonuniform grids is the high condition number of the associated system of equations. This is inherent as the grid spacing varies from smaller to bigger values rendering great deviations to the accompanying coefficients. Although a detailed analysis of the same has been avoided in this thesis, it could be inferred that the schemes advocated here are not oblivious to the same.

For steady schemes, it is further inferred that the under-relaxation parameter is important for the convergence of algebraic systems, especially for nonlinear problems. The same is difficult to estimate apriori and convergence is accelerated with optimal choice of the parameter. In our work, not much effort could be devoted in this background.

6.4 Future scopes

- The compact schemes developed in this work to treat flow problems in both Cartesian and polar coordinates. It will be interesting to develop a numerical formulation that can overlap both of these structured grids to simulate flows for complex geometries. It is anticipated that the main challenge associated with such an implementation could be to appropriately interpolate data from one set of grids to another in the overlapping section.

- It would be interesting to see whether our scheme on 3D Cartesian coordinate system can be extended for transient cases to simulate fluid flows on nonuniform grid. Here, we feel mitigating increased computational cost is the issue at hand.

- Flow around bluff bodies are simulated only for the case of stationary cylinder (square and circular). We would be interested to carry forward our schemes to compute fluid and heat flows for rotating cylinders and for cylinders which are allowed to move in traverse and horizontal direction. The associated grid transformations, wherever necessary, shall require careful formulation and implementation.

- It should be an interesting experience to extend our scheme for polar coordinates to general curvilinear coordinate system for problems involving geometries other than circular. This topic being hitherto lesser explored, allied difficulties and novelties remain unknown.
- Future aspects of the work also involve implementation of the schemes developed for real-time problems. Such an execution shall require a thorough discussion of issues pertinent to specific problem involved.