SOLUTION TO NAVIER - STOKES EQUATION IN STRETCHED COORDINATE SYSTEM

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SOLUTION TO NAVIER-STOKES EQUATION IN STRETCHED COORDINATE SYSTEM

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A thesis submitted in fulfilment of the
requirements for the award of the degree of
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To my beloved family,

The lover in you who brings my dreams comes true.

To my baby Lubna, who have brought a new level of love, patience and understanding into our lives.

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ABSTRACT

Solution to Navier-Stokes equation by Splitting method in physical orthogonal algebraic curvilinear coordinate system, also termed *'stretched coordinate'* is presented. The unsteady Navier-Stokes equations with constant density are solved numerically. The linear terms are solved by Crank-Nicholson method while the non-linear term is solved by the second order Adams-Bashforth method. The results show improved in comparison of efficiency and accuracy with benchmark steady solution of driven cavity by Ghia et al. and other first order differencing schemes including splitting scheme in Cartesian coordinate system. Enormous improvements from the original Splitting method in Cartesian coordinate observed where accurate solutions are obtained in minimum 17 X 17 from 33 X 33 resolution for Re = 100, 47 X 47 from 129 X 129 resolution for Re = 400 and 65 X 65 from 259 X 259 resolution for Re = 1000.

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CHAPTER I

INTRODUCTION

1.1 Overview

Fluid dynamics essentially deals with motion of liquids and gases, which appear to be continuous in its macroscopic structure. All the variables are considered to be continuous functions of spatial coordinates and time. The Navier-Stokes equations are able to model weather or the movement of air in the atmosphere, ocean currents, water flow in a pipe, as well as many other fluid flow phenomena.

The original Navier-Stokes equations are directly simplified by an assumption of constant density. Another simplification that commonly applied in construction of computational solution is to set all changes of fluid properties with time to zero. This is called steady solution where the Navier-Stokes equations become simpler with only steady forms are considered. A problem is termed steady or unsteady depending on the frame of reference. For instance, the flow around a ship in a uniform channel is said to be steady from the passengers' point of view, but unsteady by observers on the shore. Fluid dynamicists often transform problems to frames of reference in which the flow is steady in order to simplify the problem.

Over the last three decades, the use of CFD techniques in solving fluid flow and its applications has grown from being able to model only steady single phase, low Reynolds number flows to its current level of use in a wide range of applications. This level of growth has been enhanced by the advances in computer technology which have vastly reduced the computational times for all computations and simulations as well as increasing the size of problems which can be solved.

The application of Navier-Stokes equation in solving fluid flow has also evolved throughout this period of time with numerical method as one of the most inspiring technique that been explored. Numerical methods for 2-D steady incompressible Navier-Stokes (N-S) equations are often tested for code validation on a very well known benchmark problem, the lid-driven cavity flow. Due to the simplicity of the cavity geometry, applying a numerical method on this flow problem in terms of coding is quite easy and straight forward. Despite its simple geometry, the driven cavity flow retains a rich fluid flow physics manifested by multiple counter rotating re-circulating regions on the corners of the cavity depending on the Reynolds number. In the literature, it is possible to find different numerical approaches which have been applied to the driven cavity flow problem.

Amongst the numerous studies that use different types of numerical methods on the driven cavity flow found in the literature, priority is given for comparable methods with first order accuracy discretization scheme, Reynolds number ranging from 100 to 1000 and employ either Cartesian or algebraic stretched grid only. Some of the comparison works are the Upwind scheme, first suggested by Courant, Isaacson and Rees [10], the hybrid scheme, developed by Spalding [11], the power law scheme, described by Patankar [12] and the exponential scheme , also described by Patankar[9].

Apart from that, literature review also shows that many works have been done on the Navier-Stokes equation especially for steady, highly accurate solution which can be used as accuracy comparison. Barragy & Carey [15] have used a *p*-type finite

element scheme on a 257 ×257 strongly graded and refined element mesh. They have obtained a highly accurate (Δh^8 order) solutions for steady cavity flow solutions up to Reynolds numbers of Re=12,500. Wright & Gaskell [16] have applied the Block Implicit Multigrid Method (BIMM) to the SMART and QUICK discretizations. They have presented cavity flow results obtained on a 1024 ×1024 grid mesh for Re < 1,000. Liao & Zhu [17], have used a higher order streamfunction-vorticity boundary element method (BEM) formulation for the solution of N-S equations. They have presented solutions up to Re=10,000 with grid mesh of 257 ×257. Ghia et. al. [1] have applied a multi-grid strategy to the coupled strongly implicit method. They have presented solutions for Reynolds numbers as high as Re=10,000 with meshes consisting of as many as 257 ×257 grid points. Results by Ghia et. al. has frequently used as the benchmark solution of cavity flow.

The use of Curvilinear Grids, also termed Body Fitted Coordinates (BFC), allows the physical domain to be accurately fitted for a large number of cases. The mapping of these grids onto their topologically equivalent Cartesian mesh, with the associated mapping of the transport equations, extends the class of problems to which the numerical method technique can be applied. A similar methodology, in which the transformation to a computational domain is implicit in the discretisation techniques, has been used by Demirdzic and Peric [7] and many other researchers to solve problems with moving boundaries. The problems with this type of approach are that the use of BFC meshes increases the storage requirements and adds considerably to the complexity of the equations being solved. The approximations made to calculate the various terms become significantly more difficult to calculate. This commonly leads to further approximations being made and as a consequence errors become significant if the physical grid differs substantially from the computational Cartesian mesh.

Since this current work is only concern on square driven cavity, algebraic orthogonal curvilinear coordinate or simply termed, 'Stretched Coordinate' is used. Stretched coordinate is selected because it enables direct usage of mathematical models

derived in Cartesian coordinate with minimum verifications of the discretization methods. Stretched coordinate also enables mesh clustering that serves very well for lid-driven cavity problem. Further explanation on the advantages of having stretched grid is discussed in section 2.5.

In two dimensional solution of viscous incompressible flow, the pressure term can be eliminated by taking the cross derivative of the momentum equation. The pressure term can also be taken under consideration by velocity-pressure coupling techniques. Some of the popular velocity-pressure coupling methods are Artificial Compressibility method, Fractional-Step method and Pressure Poisson Equation method. The most commonly used velocity-pressure coupling technique is SIMPLE (Semi-Implicit Method for Pressure-Linked Equation). This technique is found to be inefficient since it involve major convergence iteration in determining the pressure values for every main velocity-time iteration. As an alternative, Karniadakis [2] had introduced a new formulation for high-order time-accurate splitting scheme for the solution of the incompressible Navier-Stokes equations.

The pressure in incompressible flow plays a very important particular role as it should always be in equilibrium with the time-dependent divergence-free velocity field, but it does not appear explicitly in the equation imposing such a divergence condition. While it is clear that the governing equation for pressure is a Poisson equation derived from the momentum equation by requiring incompressibility, it is less clear what boundary conditions the pressure should be subject to. In particular, it was argued that in the absence of singularities as time approaching zero value, property derived Neumann and Dirichlet boundary conditions lead to the same solution. However, Neumann boundary conditions are more general and always provide a unique solution for time approaching zero.

In Splitting method which is the method used in this current work, the pressure satisfies a Poisson equation with compatible Neumann boundary conditions. The exact

form of this boundary condition is very important not only because it directly affect the overall accuracy of the scheme, but also because it determines the accuracy of the time-stepping algorithm. This is particularly true in simulations of unsteady flows in complex geometry, where a separately solvable second-order pressure equation is still the only affordable approach. In this current work, splitting led to first order accuracy, so that very small time increment steps are required in order to prevent significant time differencing and splitting errors.

In particular, improved pressure boundary conditions of high order in time are introduced for minimum effect of erroneous numerical boundary. A new family of stiffly stable schemes is employed in mixed explicit/implicit time integration rules. These schemes exhibit much broader stability regions as compared to traditional Adam-family schemes. The stability properties remain almost constant as the accuracy of the integration increases, so that robust third or higher order time accurate schemes can readily be constructed.

1.2 Objective

A recent attempt to implement Splitting method introduced by Karniadakis et. al [2] in algebraic orthogonal curvilinear coordinate is motivated by the necessity to obtain more accurate and efficient first order accuracy solution of Navier-Stokes equation. First order accuracy scheme is the simplest scheme required for unsteady solution of Navier-Stokes equation. Since efficiency is the most commanding issue in unsteady solution, it is always worthwhile to have less time consuming scheme without sacrificing the accuracy of the solution.

The current work is meant to bring together the advantage of Splitting method as pressure-velocity solver of higher efficiency with the advantage of consuming

stretched grid which produce more accurate results in relatively equal number of grid points as compared to Cartesian grid.

The main objectives of the current work can be arranged in more perceptible agreement as below:

i. To develop less mesh sensitive and more efficient numerical Algorithm for unsteady two-dimensional incompressible Navier-Stokes equation.

ii. To introduce Splitting as velocity-pressure coupling method on physical orthogonal algebraic curvilinear coordinates, also termed *'stretched coordinate'* in solving Navier-Stokes equation.

iii. To study the behavior of the developed algorithm in terms of time efficiency, mesh sensitivity, accuracy and its robustness.

iv. To compare the results obtained with previously published results for the traditional driven cavity problem.

CHAPTER II

NUMERICAL SOLUTION TECHNIQUES

2.1 Introduction to Splitting method

In two dimensional solution of viscous incompressible flow, the pressure term can be eliminated by taking the cross derivative of the momentum equation. The pressure term can also be taken under consideration by velocity-pressure coupling techniques. Some of the popular velocity-pressure coupling methods are Artificial Compressibility method, Fractional-Step method and Pressure Poisson Equation method.

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2.2 *Mathematical preliminaries*

Consider a Newtonian flow with constant material properties, including constant density, governed by the Navier-Stokes and continuity equations. The Navier-Stokes equations for constant density flow, in vector form, are

$$\rho\left(\frac{\partial \vec{v}}{\partial t}+\vec{v}\cdot\nabla\vec{v}\right)=-\nabla p+\mu\nabla^2\vec{v}, \qquad 2.2.1$$

where

$$\vec{v}=u\vec{i}+v\vec{j}+w\vec{k} \qquad 2.2.2$$

is the velocity vector, p is the pressure, μ is dynamic viscosity, ρ is fluid density, and t is time.

The continuity equation for constant density is

$$\nabla\cdot\vec{v}=0 \qquad 2.2.3$$

Consider two-dimensional flow in a rectangle of height, H, and length, L. Dimensionless variables are defined as

$$\tilde{u} = \frac{u}{U},$$
$$\tilde{v} = \frac{v}{U},$$
$$\tilde{p} = \frac{p}{\rho u^2}, \qquad 2.2.4$$
$$\tilde{x} = \frac{x}{L},$$
$$\tilde{y} = \frac{y}{H}$$

where U is a reference velocity. For the present results, U is the constant velocity on the top boundary. Dropping the circumflex, the resulting dimensionless equations are

$$\frac{\partial \vec{u}}{\partial t} + \vec{v} \cdot \nabla \vec{v} = -\nabla p + \frac{1}{R_e} \nabla^2 \vec{v} \qquad 2.2.5$$

where R_e is the Reynolds number, defined as

$$R_e = \frac{UL}{v}. \qquad 2.2.6$$

In component form for both Cartesian and stretched coordinates, these equations are

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{1}{\gamma} v\frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + \frac{1}{R_e}\left(\frac{\partial^2 u}{\partial x^2} + \frac{1}{\gamma^2}\frac{\partial^2 u}{\partial y^2}\right)$$
$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + \frac{1}{\gamma} v\frac{\partial v}{\partial y} = -\frac{\partial p}{\partial y} + \frac{1}{R_e}\left(\frac{\partial^2 v}{\partial x^2} + \frac{1}{\gamma^2}\frac{\partial^2 v}{\partial y^2}\right) \qquad 2.2.7$$

where $\gamma = \frac{H}{L}$. Note that $\gamma = 1$ for our specific case of square cavity problem.

The boundary conditions are the no-penetration condition, $\vec{v} \cdot \vec{n} = 0$, where $\vec{n}$ is a unit vector normal to the boundary, and the no-slip condition, $\vec{v} \cdot \vec{\tau} = 0$, where $\vec{\tau}$ is a unit vector tangent to the boundary. For our specific traditional cavity case, the tangential velocity is $u(x) = 1$, where $0 < x < 1$.

2.3 Temporal integration and splitting of the Navier-Stokes equations

The temporal integration of the Navier-Stokes system is achieved using a semi-implicit splitting method, similar to the method of Karniadakis et. al [2] and others. Consider the Navier-Stokes expression below

$$\frac{\partial \vec{v}}{\partial t} + \vec{N}(\vec{v}) = -\nabla p + \frac{1}{R_e}\vec{L}(\vec{v}), \qquad 2.3.1$$

where $\vec{L}$ is the linear viscous term and $\vec{N}$ is the non-linear advective term,

$$\vec{L}(\vec{v}) = \nabla^2 \vec{v}, \qquad 2.3.2$$
$$\vec{N}(\vec{v}) = \vec{v} \cdot \nabla \vec{v}.$$

Integrate the above equation over one time step, Δt,

$$\int_k^{k+1} \frac{\partial \vec{v}}{\partial t} dt + \int_k^{k+1} \vec{N}(\vec{v}) dt = -\int_k^{k+1} \nabla p dt + \int_k^{k+1} \frac{1}{R_e}\vec{L}(\vec{v}) dt, \qquad 2.3.3$$

where k is the time step.

The first term is easily evaluated without approximation,

$$\int_k^{k+1} \frac{\partial \vec{v}}{\partial t} dt = \vec{v}^{k+1} - \vec{v}^{k}. \qquad 2.3.4$$

A semi-implicit method treats linear terms implicitly for stability, and non-linear term is achieved with the second-order Adams-Bashforth method,

$$\int_k^{k+1} \vec{N}(\vec{v}) dt = \left[\frac{3}{2}\vec{N}(\vec{v}^{k}) - \frac{1}{2}\vec{N}(\vec{v}^{k-1})\right]\Delta t \qquad 2.3.5$$

The explicit treatment of the nonlinear term avoids sampling $\vec{N}$ at the leading time step, which would result in nonlinear algebraic equations, requiring further iteration. The pressure term is treated by reversing the order of integration and differentiation, then introducing time-averaged pressure,

$$\int_k^{k+1} \nabla p dt = \nabla\left[\int_k^{k+1} p dt\right] = \nabla \overline{p}^{k+1} \Delta t. \qquad 2.3.6$$

Implicit treatment of the linear viscous term is achieved with the second-order Crank-Nicholson method,

$$\int_k^{k+1} \vec{L}(\vec{v}) dt = \frac{1}{2}\left[\nabla^2 \vec{v}^{k+1} + \nabla^2 \vec{v}^{k}\right]\Delta t. \qquad 2.3.7$$

The combined difference equation is now,

$$\vec{v}^{k+1} - \vec{v}^{k} + \left[\frac{3}{2}\vec{N}(\vec{v}^{k}) - \frac{1}{2}\vec{N}(\vec{v}^{k-1})\right]\Delta t = -\nabla \overline{p}^{k+1}\Delta t + \frac{1}{2R_e}\left[\nabla^2 \vec{v}^{k+1} + \nabla^2 \vec{v}^{k}\right]\Delta t \quad 2.3.7$$

The continuity equation is imposed at the leading time step,

$$\nabla \cdot \vec{v}^{k+1} = 0. \qquad 2.3.8$$

In splitting method, (2.3.7) is integrated numerically in three for each time step, each stage addressing the three terms independently. Two intermediate velocity fields, $\hat{\vec{v}}$ and $\hat{\hat{\vec{v}}}$, are introduced in order to achieve this. The three stages are,

$$\begin{aligned}
\hat{\vec{v}} - \vec{v}^{k} &= \left[\frac{3}{2}\vec{N}(\vec{v}^{k}) - \frac{1}{2}\vec{N}(\vec{v}^{k-1})\right]\Delta t, \\
\hat{\hat{\vec{v}}} - \hat{\vec{v}} &= -\nabla \overline{p}^{k+1}\Delta t, \qquad 2.3.9 \\
\vec{v}^{k+1} - \hat{\hat{\vec{v}}} &= \frac{1}{2R_e}\left[\nabla^2 \vec{v}^{k+1} + \nabla^2 \vec{v}^{k}\right]\Delta t.
\end{aligned}$$

In order to process the second step, the average pressure, $\overline{p}$, must be determined. The pressure is not needed for the first step, and therefore can be determined after $\hat{\vec{v}}$ .take divergence of (2.3.7) and use the continuity equation to obtain the Poisson's equation for pressure,

$$\nabla^2 \overline{p}^{k+1} = \nabla \cdot \left(\frac{\hat{\hat{\vec{v}}}}{\Delta t}\right), \qquad 2.3.10$$

where the nonlinear term is neglected.

All variables require boundary conditions, including $\vec{v}^{k+1}, \hat{\vec{v}}, \hat{\hat{\vec{v}}}$ and $\overline{p}$. The boundary conditions on $\vec{v}^{k+1}$ are the natural boundary conditions, which must be enforced at the final stage if the splitting method. Boundary conditions on $\hat{\vec{v}}$ and $\hat{\hat{\vec{v}}}$ can be chosen to enhance the numerical aspect of the method. Hence,

$$\hat{\vec{v}} \cdot \vec{k} = \hat{\hat{\vec{v}}} \cdot \vec{k} = 0 \qquad 2.3.11$$

on all boundaries.

Finally, there are no natural boundary conditions on the pressure since the value of pressure at the boundary depends on the velocity field in the neighborhood of the boundary. Pressure boundary conditions must be approximated from the governing equations. Take the normal component of (2.3.7) to get,

$$\vec{k} \cdot \nabla \overline{p}^{k+1} = \vec{k} \cdot \vec{v}^{k} - \vec{k} \cdot \vec{v}^{k+1} - \vec{k} \cdot \left[\frac{3}{2} \vec{N}(\vec{v}^{k}) - \frac{1}{2} \vec{N}(\vec{v}^{k-1}) \right] \Delta t + \frac{1}{2R_e} \vec{k} \cdot \left[\nabla^2 \vec{v}^{k+1} + \nabla^2 \vec{v}^{k} \right] \Delta t \qquad 2.3.12$$

Karniadakis [2] has shown that all the right hand side terms of above equation can be neglected for large Reynolds number, leaving,

$$\vec{n} \cdot \nabla \overline{p}^{k+1} = 0. \qquad 2.3.13$$

For that reason, Karniadakis [2] recommends higher order boundary conditions for a better approximation, especially for low Reynolds number flow.

2.4 Grid generation

The last two sections construct a system of partial differential equations as a mathematical model of cavity flow problem. The solution of this partial differential equations system can be greatly simplified by a well-constructed grid. It is also true that

a grid which is not well suited to the problem can lead to an unsatisfactory result. In some application, improper choice of grid point locations can lead to an apparent instability or lack of convergence. One of the central problems in computing numerical solutions to partial differential equations is that of grid generation.

Early work using finite difference methods was restricted to problems where suitable coordinate systems could be selected in order to solve the governing equations in that base system. As experience in computing complex flowfields was gained, general mappings were employed to transform the physical plane into a computational domain. Numerous advantages build up when this procedure is followed. In general, transformations are used which lead to a uniformly spaced grid in the computational plane while points in physical space may be unequally spaced.

Solution to lid-driven cavity flow can be improved by the use of proper grid arrangement. These are some of the requirements for the desired grid in order to maximize accuracy and efficiency of numerical solution for the lid-driven cavity flow:

- High resolution at all four boundaries since the velocity gradient is expected to be higher at these regions.
- Higher resolution at all corners since secondary vortices are expected to develop at these locations.
- Less resolution at the middle of the cavity since faster divergence is expected in this region.

Referring to the above requirements, Cartesian coordinate is definitely not a preferable option since it illustrates a uniform grid size in which sacrifice the other requirements for the fulfillment of any single requirement listed above. Figure 2.1 below exhibit all the above requirements for a better solution of lid-driven cavity flow.

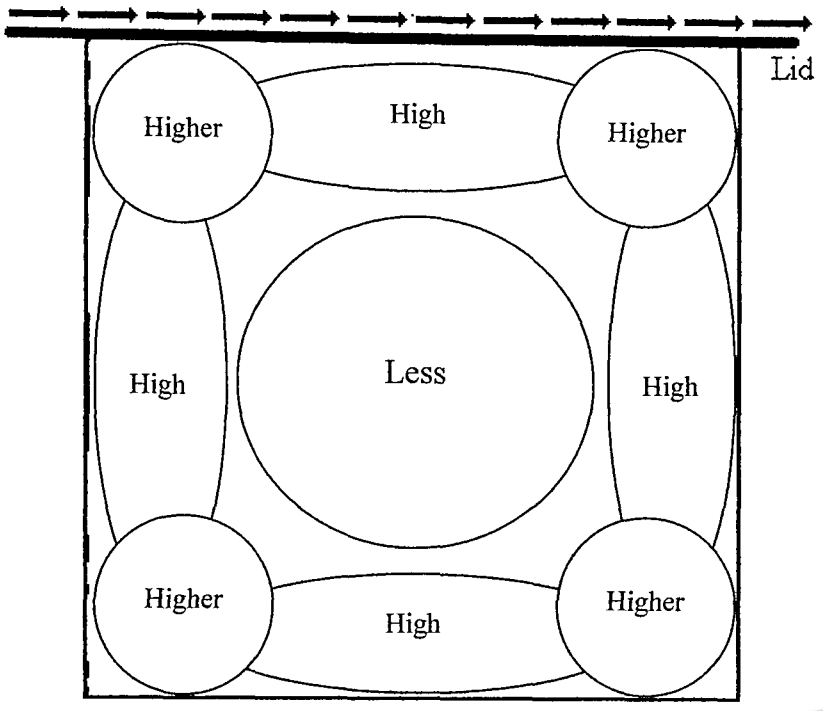


Figure 2.1: Level of resolutions suggested for lid-driven cavity flow.

2.5 *Algebraic Grid Generation Techniques*

Regular Cartesian coordinate can be 'stretched' according to the specific requirement as listed in the last section by the use of algebraic transformation technique. Algebraic grid is obtained by transforming the coordinates of every single point in regular Cartesian grid using algebraic equations. Generally, grid systems with following features are desired:

i. A mapping which guarantees one-to-one correspondence ensuring grid lines of the same family do not cross each other.

ii. Smoothness of the grid point distribution.

iii. Orthogonality of the grid lines.

iv. Options for grid point clustering.

For the case of square cavity flow, algebraic expressions are used to cluster grid points near solid boundaries and critical locations such as the corners of a cavity to provide adequate resolutions for the viscous boundary layer and secondary vortices. The main advantage of this technique is the rate at which a grid can be generated. Algebraic equations are used to relate the grid points in the computational domain to those of the physical domain. This is done by the use of interpolation scheme between the specified boundary grid points to generate the interior grid points.

Principally, flow problems where large gradients are concentrated in a specific region require refinement of resolutions on those regions. As an example, flow in the vicinity of a solid surface in a viscous fluid possesses large flow gradients. Accurate computation of flow gradients in this region requires relatively more grid points within the domain. Instead of using uniform, high resolution grid distribution in the physical domain, grid points may be clustered in the regions of high flow gradients and broaden at other regions. This technique reduces the total number of grid points and thus increases efficiency.

Refinement of mesh near walls and critical locations are done in numerous ways. In generating grid coordinate for flow in a duct, Anderson, Tannehill and Pletcher [14] derived a set of algebraic expressions to transform points in computational Cartesian coordinate to physical Stretched coordinate and vise versa. The transformation was found to be in a single horizontal direction since flow in a duct is only deals with top and bottom walls. Referring to our current objective in which to study the flow in a *square cavity,* modification of the mesh for flow in a duct is done by transforming both horizontal, x and vertical, y directions. This modification is done to create more refined mesh near all top, bottom, left and right walls of the square cavity.

The algebraic formulation for transformation between physical and computational domain is shown below:

$$\eta_1 = \alpha + (1-\alpha) + \frac{ln\{\{\beta + [(2\alpha+1)x/L] - 2\alpha\}/\{\beta - [(2\alpha+1)x/L] + 2\alpha\}\}}{ln[(\beta+1)/(\beta-1)]} \quad 2.5.1$$

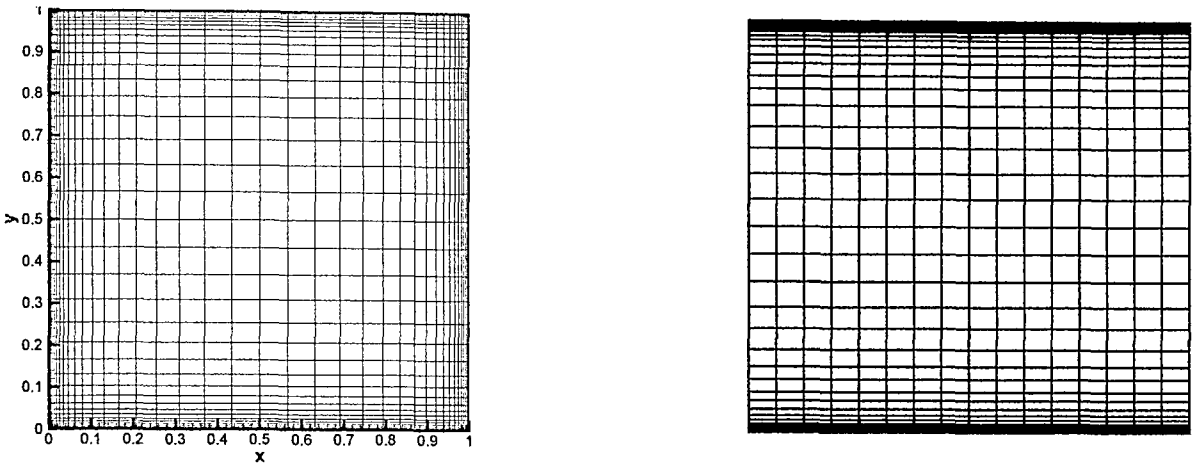
$$\eta_2 = \alpha + (1-\alpha) + \frac{ln\{\{\beta + [(2\alpha+1)y/H] - 2\alpha\}/\{\beta - [(2\alpha+1)y/H] + 2\alpha\}\}}{ln[(\beta+1)/(\beta-1)]} \quad 2.5.2$$

or inversely,

$$x = L\frac{(2\alpha+\beta)[(\beta+1)/(\beta-1)]^{(\eta_1-\alpha)/(1-\alpha)} + 2\alpha - \beta}{(2\alpha+1)\{1+[(\beta+1)/(\beta-1)]^{(\eta_1-\alpha)/(1-\alpha)}\}} \quad 2.5.3$$

$$y = H\frac{(2\alpha+\beta)[(\beta+1)/(\beta-1)]^{(\eta_1-\alpha)/(1-\alpha)} + 2\alpha - \beta}{(2\alpha+1)\{1+[(\beta+1)/(\beta-1)]^{(\eta_1-\alpha)/(1-\alpha)}\}} \quad 2.5.4$$

For a cavity of width L and height H, where β is the clustering parameter, and α defines where the clustering takes place. When α = 0 the clustering is at x=L and y=H; whereas when α =1/2 clustering is distributed equally at the four sides of the cavity. Figure 2.2 (a) shows stretched grid for square cavity (at α=1/2,β=1.25) and for further analysis, these relationship can also be modified for specific cases like turbulent channel flow (at α=0,β=1.001) as shown in Figure 2.2 (b). Figure 2.3 shows the computational domain, (η_1, η_2).



(a) Square cavity flow (b) Channel flow

Figure 2.2: Stretched grid in physical computational domains.

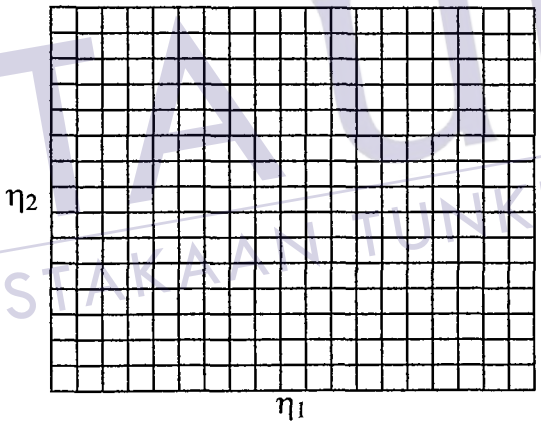


Figure 2.3: Computational domain.

For many applications, algebraic models provide a reasonable grid system with continuous and smooth matrix distributions. However, if grid smoothness, skewness, and orthogonality are of concern, grid systems generated by solving PDEs must be used. These options include elliptic, parabolic, or hyperbolic grid generators. Algebraic techniques are used not only to generate grid points for which the equations of fluid motion are solved, but they may also be used as an initial grid point distribution to start an iterative solution procedure for elliptic grid generators.

As conclusions of this section, the advantages of the algebraic 'stretched' grid generation methods are:

(1) The transformation procedure is simple and efficient.

(2) Numerical errors are minimized since matrix may be evaluated analytically.

(3) Possibility of clustering grid points in different regions.

2.6 Discretization method

The finite difference approach is the most popular discretization technique, due to its simplicity. Finite difference approximations of derivatives are obtained by using truncated Taylor series. Consider the following Taylor expansions

$$u(x+\Delta x) = u(x) + \Delta x \frac{\partial u}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2} + \frac{\Delta x^3}{6}\frac{\partial x^3 u}{\partial x^3} + \upsilon(\Delta x^4) \qquad 2.6.1$$

$$u(x-\Delta x) = u(x) - \Delta x \frac{\partial u}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2} - \frac{\Delta x^3}{6}\frac{\partial x^3 u}{\partial x^3} + \upsilon(\Delta x^4) \qquad 2.6.2$$

The first order derivative is given by the following approximations:

From (2.6.1): Forward Difference

$$\frac{\partial u}{\partial x} = \frac{u(x+\Delta x) - u(x)}{\Delta x} + \upsilon(\Delta x) \qquad 2.6.3$$

From (2.6.2): Backward Difference

$$\frac{\partial u}{\partial x} = \frac{u(x) - u(x-\Delta x)}{\Delta x} + \upsilon(\Delta x) \qquad 2.6.4$$

By substracting (2.6.1) - (2.6.2): Centered Difference

$$\frac{\partial u}{\partial x} = \frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x} + \upsilon(\Delta x^2) \qquad 2.6.5$$

An approximation for the second order derivative is gain by adding (2.6.1) + (2.6.2):

$$\frac{\partial^2 u}{\partial x^2} = \frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{\Delta x^2} + \upsilon(\Delta x^2) \qquad 2.6.6$$

The terms $\upsilon(\Delta x)$ and $\upsilon(\Delta x^2)$ indicate the remainders which are truncated (*truncation error*) to obtain the approximate derivatives. The centered difference approximation given by (2.6.5) is more precise than the forward difference (2.6.3) or the backward difference (2.6.4) because the truncation error is of higher order, a consequence of cancellation of terms of the expansions when taking the difference between (2.6.1) and (2.6.2). Since the centered difference involves both neighboring points, there is more *balanced* information on the local behavior of the function. If a better approximation is needed, one could either reduce the size of the mesh or add

more information by including higher order neighbors. It is a good exercise to derive an expression for the second order derivative including five points instead of three. Besides (2.6.1) and (2.6.2) we also need the expansions for $u(x + 2\Delta x)$ and $u(x - 2\Delta x)$:

$$u(x+2\Delta x) = u(x) + 2\Delta x\frac{\partial u}{\partial x} + \frac{4\Delta x^2\partial^2 u}{2\partial x^2} + \frac{8\Delta x^3}{6}\frac{\partial^3 u}{\partial x^3} + \frac{16\Delta x^4}{24}\frac{\partial^4 u}{\partial x^4} + \frac{32\Delta x^5}{120}\frac{\partial^5 u}{\partial x^5} + \upsilon(\Delta x^6) \qquad 2.6.7$$

$$u(x-2\Delta x) = u(x) - 2\Delta x\frac{\partial u}{\partial x} + \frac{4\Delta x^2\partial^2 u}{2\partial x^2} - \frac{8\Delta x^3}{6}\frac{\partial^3 u}{\partial x^3} + \frac{16\Delta x^4}{24}\frac{\partial^4 u}{\partial x^4} - \frac{32\Delta x^5}{120}\frac{\partial^5 u}{\partial x^5} + \upsilon(\Delta x^6) \qquad 2.6.8$$

The final result is an approximation of order $u(\Delta x^4)$

$$\frac{\partial u}{\partial x} \approx \frac{-u(x+2\Delta x) + 8u(x+\Delta x) - 8u(x-\Delta x) + u(x-2\Delta x)}{12\Delta x} \qquad 2.6.9$$

Equation (2.6.9) is an improvement of the forward difference and a symmetrical expression can be derived for the backward difference. In order to simplify the notation, when convenient we will label the discretization points with appropriate indices. With, $\Delta x^2 = h^2$ Eq. (2.6.6) becomes

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u(i+1) - 2u(i) + u(i-1)}{h^2} \qquad 2.3.11$$

Until now, we have assumed a regular Cartesian grid with uniform mesh intervals, for the derivation of finite difference approximations. In this current work, it is necessary to discretize the equations on the irregular grid of stretched grid. Consider a non-uniform 1-D discretization, for example. If finite difference approximations are sought at the grid point *i*, we can use the following Taylor expansions:

$$u(i+1) = u(i) + \frac{h_i \partial u}{\partial x} + \frac{h_i^2 \partial^2 u}{2\partial x^2} + \frac{h_i^3 \partial^3 u}{6\partial x^3} + \upsilon(h_i^4) \qquad 2.6.12$$

$$u(i-1) = u(i) - \frac{h_{i-1} \partial u}{\partial x} + \frac{h_{i-1}^2 \partial^2 u}{2\partial x^2} - \frac{h_{i-1}^3 \partial^3 u}{6\partial x^3} + \upsilon(h_{i-1}^4) \qquad 2.6.13$$

The forward and backward difference approximation for the first order derivative can be assembled as before. An expression which involves both $u(i\text{-}1)$ and $u(i\text{+}1)$ is obtained from (2.6.12) - (2.6.13) as

$$\frac{\partial u}{\partial x} \approx \frac{u(i+1) - u(i-1)}{h_i + h_{i-1}} \qquad 2.6.14$$

Notice that the terms corresponding to the second order derivatives in the Taylor expansions do not cancel exactly, as in the case of the centered difference in (2.6.5) due to the nonuniformity of the mesh intervals, therefore we have a larger truncation error.

It is often convenient to involve the mid-points of the mesh intervals, indicated as i - ½ and i + ½, to express first order derivatives, as

$$\frac{\partial u}{\partial x} \approx [u(i+\frac{1}{2}) - u(i-\frac{1}{2})]/(\frac{h_i + h_{i-1}}{2}) \qquad 2.6.15$$

This result can be useful to obtain an approximation for the second order derivative on the nonuniform mesh. We can write

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x}(\frac{\partial u}{\partial x}) \approx [\frac{\partial u}{\partial x}|_{i+\frac{1}{2}} - \frac{\partial u}{\partial x}|_{i-\frac{1}{2}}]/(\frac{h_i + h_{i-1}}{2}) \qquad 2.6.16$$

We can then express $\partial u / \partial x \mid_{i+½}$ and $\partial u / \partial x \mid_{i-½}$ with centered differences, which are of order $U(h^2)$, and obtain

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x}(\frac{\partial u}{\partial x}) \approx [\frac{u_{i+1} - u_i}{h_i} - \frac{u_i - u_{i-1}}{h_{i-1}}](\frac{2}{h_i + h_{i-1}}) \qquad 2.6.17$$

CHAPTER V

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