Computation of Heat and Fluid Flow using Domain Decomposition Method

A Project Report Submitted in Partial Fulfillment of the Requirements for the Degree of

Bachelor of Technology

by

Parmar Harsharajsinh Birendrasinh

and

Rohan Agrawal



to the

DEPARTMENT OF MECHANICAL ENGINEERING INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI GUWAHATI - 781039, ASSAM

MAY 2019

Dedicated to our parents for their unconditional love and support.

CERTIFICATE

This is to certify that the work contained in this thesis entitled "Computation of Heat and Fluid Flow using Domain Decomposition Method" is a bonafide work of Parmar Harsharajsinh Birendrasinh and Rohan Agrawal carried out in the Department of Mechanical Engineering, Indian Institute of Technology Guwahati under my supervision and that it has not been submitted elsewhere for a degree.

Supervisor: Dr.Madhusudhana R.Gavara

Assistant Professor, Department of Mechanical Engineering, Indian Institute of Technology Guwahati, Assam.

May, 2019 Guwahati.

APPROVAL SHEET

This project report entitled "Computation of Heat and Fluid Flow using Domain Decomposition Method", a bonafide work by Parmar Harsharajsinh Birendrasinh and Rohan Agrawal is approved for the degree of Bachelor of Technology.

Examiners

Supervisor

Chairman

Department of Mechanical Engineering, Indian Institute of Technology Guwahati, Assam.

May, 2019 Guwahati.

i

DECLARATION

I declare that this written submission represents my ideas in my own words and where others' ideas or words have been included, I have adequately cited and referenced the original sources. I also declare that I have adhered to all principles of academic honesty and integrity and have not misrepresented or fabricated or falsified any idea/data/source in my submission. I understand that any violation of the above will be cause for disciplinary action by the Institute and can also evoke penal action from the sources which have thus not been properly cited or from whom proper permission has not been taken when needed.

> Parmar Harsharajsinh Birendrasinh 150103051

> > Rohan Agrawal 150103058

> > > May 16, 2019

Abstract

This project is aimed to develop and parallelize CFD solvers for incompressible heat and fluid flows. The solver for incompressible heat and fluid flows is based on spectral method. The parallelization of these codes is done based on the domain decomposition method using OpenMP. This project is mainly divided into two modules - developing spectral codes and parallelization of FDM and spectral codes. FDM codes are parallelized to lay the foundation for working on spectral codes for fluid flow and heat transfer.

In the first module, a solver is developed for conduction heat transfer problems. The solver is validated using heat conduction problem for which analytical solution is available. Then, a solver for fluid flow problems is developed and the solver is validated against channel flows and lid driven cavity. Then the solver is extended for convective heat transfer and the solver is validated for forced convection in lid driven cavity and natural convection in differentially side heated cavity. The above solvers are for regular rectangular geometries. A solver also is developed for conduction in a triangular solid plate and is validated successfully.

In the second module, parallelization of the codes for heat transfer and fluid flow is carried out. This module consists of two parts involving parallelization of codes based on FDM and spectral methods respectively. First, one dimensional and two dimensional heat conduction problems are implemented by dividing the domain into smaller domains. The computation of individual smaller domains is given to different processors. The parallelization is further extended to channel flow and lid driven cavity problem. In these conduction problems for 1-D and 2-D, the discretization is carried out using both FDM and spectral methods. For fluid flow problems the discretization is carried out using spectral methods.

Acknowledgement

We have diligently worked towards the accomplishment of the desired goals in this project however, it would not have been possible without positive feedback and inputs from colleagues and mentors. We would like to express our sincere thanks to all of them.

We would like to pay high regards to our supervisor Dr. Madhusudhana. R. Gavara for his numerous valuable insights and guidance whenever it seemed like we were getting fixated on a problem or deviating from our path.

We would also like to thank the supervising panel for their constructive judgements and for suggesting enhancements in our algorithm. Their feedback on the results and validation was instrumental in pushing our cognitive skills for performing on a high level of quality.

Finally, our sincere thanks also goes to our colleagues and everyone who has directly or indirectly contributed to this work by suggesting references and novel ideas which gave us alternative insights into our work.

Contents

Li	st of	Figure	es	v
Li	st of	Tables	5	viii
1	Intr	oducti	ion	1
	1.1	Parall	el Computing	2
		1.1.1	Parallel Computing Memory Architecture	2
		1.1.2	Important Terms	4
	1.2	Spectr	al Methods	5
	1.3	Litera	ture Review	6
	1.4	Curren	nt Emphasis	7
	1.5	Proble	ems Solved	7
	1.6	Organ	ization of The Report	8
2	CFI	D Com	putations using Spectral Methods	9
	2.1	Mathe	ematical Treatment	9
		2.1.1	Governing Equations	9
		2.1.2	Spatial Discretization	10
		2.1.3	Temporal Discretization	12
		2.1.4	Treatment for Triangular domains	14
	2.2	Two I	Dimensional Heat Conduction	16

		2.2.1	Physical System	16
		2.2.2	Results and Validation	17
	2.3	Chann	nel Flow	20
		2.3.1	Physical System	20
		2.3.2	Results	21
	2.4	Lid-dr	iven Square Cavity	22
		2.4.1	Physical System	22
		2.4.2	Results and Validation	24
	2.5	Natur	al Convection	30
		2.5.1	Physical System	30
		2.5.2	Results	31
	2.6	Heat (Conduction: Triangular Domain	32
		2.6.1	Physical System	32
		2.6.2	Results	34
3	Para	2.6.2 alleliza	Results	34 35
3	Par 3.1	2.6.2 alleliza 1D He	Results	34 35 35
3	Par 3.1	2.6.2 alleliza 1D He 3.1.1	Results	34 35 35 36
3	Par 3.1	2.6.2 alleliza 1D He 3.1.1 3.1.2	Results	34 35 36 36
3	Par 3.1 3.2	2.6.2 alleliza 1D He 3.1.1 3.1.2 2D He	Results	34 35 36 36 36 39
3	Par . 3.1 3.2	2.6.2 alleliza 1D He 3.1.1 3.1.2 2D He 3.2.1	Results	34 35 36 36 39 40
3	Par 3.1 3.2	2.6.2 alleliza 1D He 3.1.1 3.1.2 2D He 3.2.1 3.2.2	Results	34 35 36 36 39 40 42
3	Par 3.1 3.2 Par	2.6.2 alleliza 1D He 3.1.1 3.1.2 2D He 3.2.1 3.2.2 alleliza	Results	34 35 36 36 39 40 42 45
3	Par. 3.1 3.2 Par. 4.1	2.6.2 alleliza 1D He 3.1.1 3.1.2 2D He 3.2.1 3.2.2 alleliza One D	Results	34 35 36 36 39 40 42 42 45
3	Par. 3.1 3.2 Par. 4.1	2.6.2 alleliza 1D He 3.1.1 3.1.2 2D He 3.2.1 3.2.2 alleliza One D 4.1.1	Results	34 35 36 36 39 40 42 42 45 45
3	Par. 3.1 3.2 Par. 4.1	2.6.2 alleliza 1D He 3.1.1 3.1.2 2D He 3.2.1 3.2.2 alleliza One D 4.1.1 4.1.2	Results	34 35 36 36 39 40 42 42 45 45 45 45

References				73
	5.1	Future	Scope	72
5	Con	clusio	ns	71
		4.4.2	Domain Decomposition with Four Subdomains	67
		4.4.1	Domain Decomposition with Two Subdomains	64
	4.4	Lid Dr	riven Cavity	64
		4.3.2	Domain Decomposition with Four Subdomains	59
		4.3.1	Domain Decomposition with Two Subdomains	56
	4.3	Chann	el Flow	56
		4.2.2	Domain Decomposition with Four Subdomains	51
		4.2.1	Domain Decomposition with Two Subdomains	48

List of Figures

1.1	Shared Memory	3
1.2	Distributed Memory	3
1.3	Hybrid Memory	4
2.1	2D Heat conduction	16
2.2	Temperature contours	18
2.3	Mid-line profile comparison	18
2.4	2D Channel flow	20
2.5	Velocity vectors	22
2.6	Lid-driven cavity	23
2.7	Steady state streamlines comparison for $Re = 100, 400$	27
2.8	Steady state streamlines comparison for $Re = 1000, 2000$	28
2.9	Variation of velocity along the center-line of the driven cavity for different Re	29
2.10	Natural convection in a square cavity	30
2.11	Comparison of streamfunction contours [a,b] and isotherms [c,d] for $Ra = 10^7$	32
2.12	Heat conduction in a triangular plate	33
2.13	Isotherms for the triangular plate	34
3.1	1D Heat conduction	35
3.2	Temperature distribution using Jacobi method	37
3.3	Temperature distribution using domain decomposition	39

3.4	2D Heat conduction	40
3.5	TDMA line-by-line method [Patankar [1]]	40
3.6	Temperature distribution using TDMA sweeps	41
3.7	Temperature distribution using domain decomposition	43
4.1	1D Heat conduction	46
4.2	2D Heat conduction - two subdomains	48
4.3	Midline profile comparison	50
4.4	Temperature contour plot for two subdomains	51
4.5	2D Heat conduction - four subdomains	52
4.6	Vertical midline profile comparison	54
4.7	Horizontal midline profile comparison	54
4.8	Temperature contour plot for four subdomains	55
4.9	Channel flow - two subdomains	57
4.10	Combined grid layout for two subdomains	57
4.11	Velocity vectors for channel flow with two subdomains $\ldots \ldots \ldots \ldots$	59
4.12	Channel flow - four subdomains	60
4.13	Combined grid layout for four subdomains	61
4.14	Velocity vectors for channel flow with four subdomains $\ldots \ldots \ldots \ldots$	63
4.15	Lid driven cavity - two subdomains	65
4.16	Velocity vectors for lid driven flow at $Re = 10$	67
4.17	Lid driven cavity - four subdomains	68

List of Tables

2.1	Comparison of flow variable M_1 for the square driven cavity at $Re = 100$	25
2.2	Comparison of flow variable M_2 for the square driven cavity at $Re = 100$	25
2.3	Comparison of flow variable M_1 for the square driven cavity at $Re = 400$	26
2.4	Comparison of flow variable M_2 for the square driven cavity at $Re = 400$	26
3.1	Jacobi iterative method	36
3.2	Domain decomposition with two subdomains	37
3.3	Domain decomposition with four subdomains	38
3.4	TDMA sweeps method	41
3.5	2D domain decomposition with two sub-domains	42
4.1	Comparison of serial, parallel times and speed-up over various grid sizes for	
	1D conduction.	47
4.2	Comparison of serial, parallel times and speed-up over various grid sizes for	
	2D conduction with two subdomains	51
4.3	Comparison of serial, parallel times and speed-up over various grid sizes for	
	2D conduction with four subdomains	55
4.4	Comparison of serial, parallel times and speed-up over various grid sizes for	
	channel flow with two subdomains. \ldots . \ldots . \ldots . \ldots . \ldots	59
4.5	Comparison of serial, parallel times and speed-up over various grid sizes for	
	channel flow with four subdomains.	63

4.6	Comparison of serial, parallel times and speed-up over various grid sizes for	
	lid driven cavity with two subdomains	66
4.7	Comparison of serial, parallel times and speed-up over various grid sizes for	
	lid driven cavity with four subdomains	70

Nomenclature

- α Thermal Diffusivity
- \dot{S}_{gen} Source term
- ϵ Convergence limit

 $\hat{u}_k(t)$ time dependant expansion spectral coefficients

- ν Kinematic Viscosity
- ω vorticity
- ψ stream function
- ρ Density
- \tilde{V} non-dimensional intermediate velocity vector at time $(n+1)\Delta t$
- b_x Body force in x-direction
- b_y Body force in y-direction
- c_i coefficients to evaluate first derivative matrix $D^{(1)}$
- c_p Specific heat capacity at constant pressure
- $D^{(1)}$ Chebeyshev collocation first derivative matrix
- $D_{ik}^{(1)}$ coefficients of matrix $D^{(1)}$

Gr	Grashof	Number

- $h_i(x)$ Lagrange polynomials
- *k* Thermal Conductivity
- N number of collocation points in x
- P non-dimensional pressure field

p Pressure

- Pr Prandtl Number
- Q Heat flux
- T Temperature
- t Time
- $T_k(x)$ Chebyshev polynomials of order k
- u Velocity component in the x-direction
- $u_N(x,t)$ Polynomial approximation of degree N
- V non-dimensional velocity vector
- v Velocity component in the y-direction
- x_i Chebyshev-Gauss-Lobatto points

Chapter 1

Introduction

Fluid flow and heat transfer are the central phenomena governing various physical processes. Their understanding and visualization is important for designing components ranging from micro-scale fuel cells to commercial power systems. Experimental and numerical approaches serve to resolve the flow fields in various situations with each having their own benefits. From an overall perspective, experiments and computations go hand-in-hand and complement each other. In designing systems, computations are first carried out to consider numerous variations and then experiments follow up to characterize their performance. On the other hand for understanding novel flows, experiments precede computations to give insights on their characteristics [1].

Numerical methods for solving PDEs have been developed since the 1950s with first introductions to Finite Difference methods (FDM) [2]. Since then many more methods have been devised with broader applications in fluid mechanics, structural analysis and other diverse fields. Finite element method (FEM), Finite Volume method (FVM) and Spectral methods have been used recently for solving flows. The FDM, FVM and FEM are local methods and have a limited order of accuracy (2^{nd} or 3^{rd} order) promoting the need for high accuracy solution methods. The present work fills this gap and focuses on formulating high-accuracy Chebyshev Spectral codes for solving certain fundamental fluid flow and heat transfer problems.

Traditional serial computing proves to be insufficient and may not be able to solve such problems in reasonable time. In some situations large number of parametric studies need to be performed to find the appropriate and optimal design values. In such applications the use of multiple processors becomes essential to solve the problem in reasonable time. To facilate the use of multiple processors to work concurrently on different tasks of the same problem parallelization of the code is essential.

1.1 Parallel Computing

Parallel computing in its simplest sense is to make use of multiple computing resources which may include multi-core processors or multi-processors inteconnected via a communication network to solve complex computational problems which can be broken down into multiple discrete pieces concurrently. Each part is then broken down to a set of instructions which are then run on individual processor (Computing resource). Parallel computing can therefore combine multiple resources to achieve high performance and very fast computing.

There are different ways to make use of computing resources concurrently which define the different parallel computing architectures.

1.1.1 Parallel Computing Memory Architecture

Parallel computing memory architectures can be broadly classified as shared , distributed and hybrid distributed-shared memory architectures.

• Shared Memory In shared memory parallel computers all processors have access to all memory as global address space. Multiple processors can share the same memory resources while operating independent of each other. Changes in a memory location effected by one processor are visible to all other processors. This leads to two problems which needs to be addressed while designing a shared memory system: Performance degradation due to contention. Coherence problem. Shared memory architecture can further be classified as Uniform Memory Access (UMA) and Non-Uniform Memory Access (NUMA).



Fig. 1.1: Shared Memory

• Distributed Memory In distributed memory computers processors have their own local memory which means there is no concept of global address space. Since memory in one processor doesn't map to another processor changes made by one are not visible to the other. Therefore to communicate and synchronise data between inter-processor memory a communication network is required which can vary widely and can simply be ethernet. It becomes the responsibility of the programmer to define how data communication and synchronisation between tasks take place.



Fig. 1.2: Distributed Memory

• Hybrid Distributed-Shared Memory Hybrid distributed-shared memory architecture employs both shared and distributed memory architectures. The shared memory component can be a shared memory machine and/or graphics processing units (GPU) while the distributed memory component is the networking of multiple shared memory/GPU machines. Therefore, a network communications is required to communicate data and synchronise tasks between machines participating in the system.



Fig. 1.3: Hybrid Memory

For our present work, we are working with shared memory architecture using the OpenMP library to parallelize the codes.

1.1.2 Important Terms

Here we discuss some of common terminoly associated with parallel computing to assess the efficiency and performance of the parallel codes.

- **Parallel Overhead** The time consumed in coordinating parallel tasks as opposed to doing some useful work. It may include factors such as process creation, thread forking/joining, wait for member threads, data communication and synchronization.
- Amdahl's Law Amdahl's Law states that potential program speedup is defined as the fraction of code (P) that can be parallelized: Equation for Amdahl's Law,

Speed-up =
$$\frac{1}{\frac{P}{N} + S}$$
 (1.1)

where P = parallel fraction, N = number of processors and S = serial fraction

• Observed Speed - Up Observed speedup of a code which has been parallelized is defined as the ratio of wall-clock time of serial execution to wall-clock time of parallel

execution. Equation for Observed Speed-Up,

Observed speed-up = $\frac{\text{Wall-clock time of serial execution}}{\text{Wall-clock time of parallel execution}}$ (1.2)

1.2 Spectral Methods

Spectral methods are higher-order accurate numerical methods that surfaced in solving PDEs during the late 1970. The order of accuracy is said to be equal to the number of grid points provided that the function to be approximated is smooth, analytic and non-singular. The type of approximation used for the function forms a cardinal aspect in any spectral method. On the lines of this, usually two types of Spectral methods are used in CFD:

- Fourier Spectral Methods These are used in problems exhibiting a periodicity at the boundaries
- Chebyshev Spectral Methods These are used for problems having non-periodic boundary conditions

These methods can be rendered useful particularly for regular domains and usually involve mathematical and implementation-level difficulties when extended to arbitrary domains. Our work is based on Chebyshev collocation form of spectral methods which use a pre-defined set of grid points called Gauss-Lobatto points which form a biased grid with refinements near the corners. Specifically, in case of finite domains with "physical" boundary conditions, for instance the no slip condition, polynomial basis functions (Chebyshev) lead to efficient and accurate algorithms [3]. These characteristics are to be kept in mind when using this method for practical problems.

1.3 Literature Review

Since the development of spectral methods in late 1970, a considerable amount of research has been aimed at applying them in solving high-accuracy problems. C. Canuto et al. [4] and D. Gottlieb et al. [5] considered the application of spectral methods in Direct Numerical Simulations of turbulent flows. They also categorized the preferred type of spectral method that is fourier or chebyshev depending on the boundary conditions of problems. Solomonoff et al. [6] considered the global characteristics of psuedospectral methods and highlighted the critical aspects to ensure correct solution procedure. Deville et al. [7] worked on deriving the derivative matrices for chebyshev spectral methods.

Fluid flow problems are solved by using projection methods in conjunction with spectral discretizations in this study and so a brief background on the developments on this side are considered. Botella O. et al. [8] provided solutions to the Navier-Stokes equation using a combination of spectral and temporal schemes. Chorin [9] and Temam [10] were the first ones to propose the original form of projection method and since then several variants have been devised. Huges et al. [11] were reportedly the first to use projection methods in combination with spectral methods. Finally, Streett et al. [12] applied the semi-implicit projection method to large-scale problems and also formulated a discretized version of the same.

Domain decomposition as a method for parallelization was pioneered in Computational Fluid Dynamics by Gropp et al. [13]. They highlighted the benefits of domain decomposition pertaining to its flexibility in containing adaptive refinements and its modular pathway to parallelism. A simple classical problem of flow over a backstep was solved to illustrate these features. Carvalho et al. [14] extended over this work and implemented a variation of domain decomposition using overlapping sections of the subdomains. They reported an accelerated convergence of the algorithm as a result of increased overlapping. Recent work by Nestola et al. [15] implemented overlapping domain decomposition on an immersed boundary method for fluid-structure interaction.

1.4 Current Emphasis

By virtue of their high accuracy, Spectral methods find application in scenarios where it is necessary to solve the full Navier-Stokes equation. The full-solutions contribute to enhanced understanding and knowledge about certain fundamental flow phenomena. Firstly, Direct Numerical Simulation (DNS) of turbulent flows is an important application of spectral methods. Secondly, they are also used in stability analysis where it is critical to refine the base flow accurately for applying perturbations.

Presently, we are developing spectral codes that would be solved through a parallel architecture and used for Large Eddy Simulations (LES). We have focused on developing solution schemes for incompressible flows and tested them on certain fundamental fluid flow and heat transfer problems. For parallelization, work has been done on TDMA sweeps and Domain Decomposition. The results have been validated using available analytical solutions and benchmark results in prevalent literature.

1.5 Problems Solved

The present work comprises of various test problems to validate our spectral code and they are listed as follows,

- Two-dimensional heat Conduction in a rectangular plate
- Plane Poiseuille flow
- Lid-driven flow in a square cavity
- Natural convection in a square cavity
- Two-dimensional heat conduction in a triangular plate

1.6 Organization of The Report

This chapter provides a background for parallel computing. We have provided a description of different architectures used in parallel computing. Then we described some of relevant terms to study different algorithms for parallel programs. In the first half of this report, spectral codes have been developed for solving fluid flow and heat transfer problems. The parallelization part follows the code development and is divided into two parts - parallel computing of FDM codes and parallel computing of Spectral codes.

Parallelization of FDM codes for the following problems is presented:

- One Dimensional Heat conduction
- Two Dimensional Heat conduction

Spectral codes for the following problems have been parallelized:

- One Dimensional Heat conduction
- Two Dimensional Heat conduction
- Channel flow
- Lid driven cavity

The computations proceed in a structured manner describing the governing equations, spatial and temporal discretization and special treatment demanded by triangular domains. Thereafter, the problems are considered and each one comprises of,

- Physical system description
- Governing equation under assumptions
- Results
- Conclusion

Chapter 2

CFD Computations using Spectral Methods

2.1 Mathematical Treatment

2.1.1 Governing Equations

The problems discussed in this study are confined to two dimensions and so all the dimensional form of governing equations have been expressed accordingly.

Heat Conduction

The two dimensional heat conduction equation can be represented as,

$$\rho c_p \frac{\partial T}{\partial t} = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \dot{S}_{gen}$$

Fluid flow and Heat transfer

The dimensional form of governing equations can be represented as follows.

Continuity Equation,

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

x-momentum equation,

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + b_x$$

y-momentum equation,

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) + b_y$$

Energy convection,

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \dot{S}_{gen}$$

For natural convection the governing equations change slightly and are usually expressed in their non-dimensional form. The equations that change are expressed below:

x-momentum equation,

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + Pr\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

y-momentum equation,

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + Pr\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + GrPr^2T$$

2.1.2 Spatial Discretization

The equations are spatially discretized using a Chebyshev collocation spectral method. The collocation method has a characteristic that the numerical solution is forced to satisfy governing equations exactly at the collocation points. Thereby if we wish to solve for a

function u(x,t) on the domain [-1,1] then it may be approximated as

$$u_N(x,t) = \sum_{k=0}^{N} \hat{\boldsymbol{u}}_k(t) T_k(x)$$

For the Chebyshev collocation method, $T_k(x)$ represents chebyshev polynomials of order k. The grids points serve for interpolation and are defined as the Chebyshev-Gauss-Lobatto points,

$$x_i = \cos\left(\frac{\pi i}{N}\right) \quad i = 0, 1, \dots, N$$

These points correspond to extreme points of Chebyshev polynomials of order N,

$$T_N(x) = \cos(N\cos^{-1}x)$$

The expansion coefficients, $\tilde{u}_k(t)$ may be evaluated using the inverse relation

$$\hat{\boldsymbol{u}}_{k}(t) = \frac{2}{Nc_{k}} \sum_{i=0}^{N} \frac{u_{N}(x_{i}, t)}{c_{i}} \cos\left(\frac{k\pi i}{N}\right), \quad k = 0, 1, \dots, N$$

where c_i and $c_k = 1$ for i, k = 1, 2, ..., N - 1 and $c_0 = c_N = 2$.

The interpolation in collocation spectral method can also be expressed in terms of Lagrange polynomials of order N, $h_i(x)$ such that $h_i(x) = \delta_{ik}$, the Kronecker operator. The Lagrange polynomials for the points considered may be represented by:

$$h_i(x) = \frac{(-1)^{i+1}(1-x^2)T'_N(x)}{\bar{c}_i N^2(x-x_i)}, \quad i = 0, 1, \dots, N$$

where $\bar{c}_i = 1$ for i = 1, ..., N - 1 and $\bar{c}_0 = \bar{c}_N = 2$.

The spatial derivative of $u_N(x,t)$ at the collocation points x_i is evaluated using the analytical derivatives of Lagrange polynomials,

$$u'_N(x_i, t) = \sum_{k=0}^{N} D_{ik}^{(1)} u(x_k, t), \quad i = 0, 1, \dots, N$$

where $D^{(1)}$ is the Chebyshev collocation derivative matrix. It is given by the following expression:

$$D_{ik}^{(1)} = \begin{cases} \frac{c_i(-1)^{i+k}}{c_k(x_i - x_k)}, & i \neq k, \\ -\frac{x_k}{2(1 - x_k^2)}, & 1 \le i = k \le N - 1, \\ \frac{2N^2 + 1}{6}, & i = k = 0, \\ -\frac{2N^2 + 1}{6}, & i = k = N. \end{cases}$$

The Chebyshev collocation second derivative matrix $D^{(2)}$ can be obtained by following the relation $D^{(2)} = (D^{(1)})^2$. The higher order derivatives are obtained in a similar manner that is by multiplying $D^{(1)}$ successively.

2.1.3 Temporal Discretization

Projection Method

Projection method belongs to the predictor-corrector class of algorithms and is non-iterative in nature. Pressure acts as a projection of the predicted velocity field to form a divergence free space in this class of methods. Spectral methods offer high accuracy but as is the case with most numerical schemes, there is a trade-off between accuracy and stability. This implies that spectral methods when used with ill-conditioned temporal schemes can lead to largely unstable behaviour.

We have used a second-order semi-implicit time integration scheme and in addition the
spatial discretization is carried out using a Chebyshev collocation spectral method. The time integration scheme is formed as a combination of Crank-Nicolson scheme acting on the diffusive terms and Adams-Bashforth scheme acting on the convective terms. The projection method partitions the solution of Navier-Stokes equations into two decoupled problems. An intermediate velocity field is calculated using the Burgers equation and thereafter the Poisson equation for pressure is used to correct the velocity field as to satisfy continuity. The semi-implicit projection method discussed above can be described as follows:

a) Advection-Diffusion step which involves the intermediate velocity at $(n+1)\Delta t$, \tilde{V}

$$\frac{\dot{V} - V^n}{\Delta t} = \frac{1}{Re}D(V) - NL(V) \quad \text{in} \quad \Omega$$

Boundary conditions for this intermediate velocity

$$\hat{\boldsymbol{\tau}} \cdot \tilde{V} = \hat{\boldsymbol{\tau}} \cdot V + \hat{\boldsymbol{\tau}} \cdot \Delta t (2 \boldsymbol{\nabla} P^n - \boldsymbol{\nabla} P^{n-1}) \text{ on } \partial \Omega$$

 $\hat{\boldsymbol{n}} \cdot \tilde{V} = \hat{\boldsymbol{n}} \cdot V \text{ on } \partial \Omega$

Here $NL(V) = (V \cdot \nabla)V$ and $D(V) = \nabla^2 V$ represent the advection and diffusion terms.

b) Pressure correction step solves the Poisson equation for P^{n+1}

$$\nabla^2 P^{n+1} = \frac{\boldsymbol{\nabla} \cdot \tilde{V}}{\Delta t} \quad \text{in} \quad \Omega$$

With homogeneous Neumann boundary conditions

$$\hat{\boldsymbol{n}} \cdot \boldsymbol{\nabla} P^{n+1} = 0 \quad \text{on} \quad \partial \Omega$$

Thereafter the velocities are updated as given below,

$$V^{n+1} = \tilde{V} - \Delta t \boldsymbol{\nabla} P^{n+1} \quad \text{in} \quad \Omega + \partial \Omega$$

The combination of an explicit second-order Adams-Bashforth scheme for the advection terms and an implicit Crank-Nicolson scheme for diffusion terms can be described as follows.

$$NL(V) = \frac{3}{2}NL(V^{n}) - \frac{1}{2}NL(V^{n-1})$$

$$D(V) = \frac{D(\tilde{V}) + D(V^n)}{2}$$

These expressions are used in the Burgers equation at each time step.

2.1.4 Treatment for Triangular domains

When extending spectral methods to triangular domains we transform the computational domain to represent the physical system and thereby the derivatives in the physical space and in the computations are different and related through chain rule [16].

A mapping is involved for transforming the derivatives and can be represented as given below.

 ζ, η - Physical system variables x, y - Computational domain variables

Domain Transformation

The computational and physical domains can be seen to be related in a particular way that leads to the orientation of triangle as given in the figure. This transformation can be detailed as follows:

$$\zeta = -\frac{1}{4}(1-x)(1-y) + 1$$

$$\eta = \frac{1}{2}(y-1)$$

The triangular domain so formed is given as $\{(\zeta, \eta) : 0 \leq \zeta \leq 1, -1 \leq \eta \leq 0, \zeta + \eta \geq 0\}$ mapped from the square computational domain.

The Inverse mapping is given as:

$$x = \frac{2(\zeta - 1)}{\eta + 1} + 1$$
$$y = 2\eta + 1$$

The derivatives can then be transformed and expressed as given below:

$$u_{\zeta} = \frac{2}{\eta+1}u_x$$
$$u_{\zeta\zeta} = \left(\frac{2}{\eta+1}\right)^2 u_{xx}$$
$$u_{\eta} = -\frac{2(\zeta-1)}{(\eta+1)^2}u_x + 2u_y$$
$$u_{\eta\eta} = \frac{4(\zeta-1)^2}{(\eta+1)^4}u_{xx} - \frac{8(\zeta-1)}{(\eta+1)^2}u_{xy} + \frac{4(\zeta-1)}{(\eta+1)^3}u_x + 4u_{yy}$$

So finally the laplacian in the physical coordinates can be written in terms of those in the computational domain as:

$$\Delta u = \left\{ \left(\frac{2}{\eta+1}\right)^2 + \frac{4(\zeta-1)^2}{(\eta+1)^4} \right\} u_{xx} - \frac{8(\zeta-1)}{(\eta+1)^2} u_{xy} + \frac{4(\zeta-1)}{(\eta+1)^3} u_x + 4u_{yy} \right\}$$

This transformation has been applied to a heat conduction problem in a triangular plate discussed in the subsequent sections.

2.2 Two Dimensional Heat Conduction

Heat conduction problems play an important role as preliminary tests for validating the code structure and proper running. In this case we have considered a simple steady state problem for which analytical solutions exist ensuring proper validation.

2.2.1 Physical System

The physical system consists of a square plate which has three adjacent sides at the same temperature (T_c) as shown in Fig. 2.1. The remaining side is kept at a higher temperature (T_h) and the source terms are taken to be zero giving a source-less heat diffusion through the plate.

Plate length is represented as L and width is represented as W. Constant temperatures are applied at the four edges. Thermal diffusivity of the material is assumed to be unity as it serves just a scaling factor as far as computations are concerned.



Fig. 2.1: 2D Heat conduction

The heat conduction is assumed to be steady and the effects from generation terms

have been neglected. The thermophysical properties are assumed to be independent of temperature.

Governing Equation

Under the assumption of Steady state and zero generation in the plate the governing equation reduces to a laplace equation.

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

Boundary Conditions

At the left, right and bottom wall:

$$T_c = 300 \, K$$

At the top wall:

 $T_h = 400 \, K$

2.2.2 Results and Validation

Validation of the results is carried out by comparing with analytical solution available in Holman [17], the expression of which is shown below:

$$\frac{T - T_c}{T_h - T_c} = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n+1} + 1}{n} \sin \frac{n\pi x}{W} \frac{\sinh(n\pi y/W)}{\sinh(n\pi H/W)}$$

Temperature values along a horizontal center line are calculated using the analytical expressions and plotted along with the numerical results. An infinite sequence is surfaced in the exact solution and so we have to limit it at a certain n to enable numerical computation of temperatures. Cut-off limit is set by considering the difference between successive summation series and the series is terminated when the difference goes below 10^{-12} . The plot shown in Fig. 2.3 gives the comparison along domain's horizontal mid-line.



Fig. 2.2: Temperature contours



Fig. 2.3: Mid-line profile comparison

We observe that the mid-line numerical solution plot coincides exactly with the analytical solution. This validation serves as an important check to guarantee that our solution technique can accurately tackle the most fundamental problems. So we conclude from this problem that our code can accurately handle pure diffusion and diffusion related terms in general governing equations.

2.3 Channel Flow

Code for solving Incompressible fluid flow is validated using various test case studies. The classical problems related to incompressible flows like 2D Channel flow and Lid-driven Cavity flow are simulated to examine their accuracy.

The model represents a channel formed by placing two infinite plates parallel to each other in the physical domain. A fully developed profile is used as inlet condition and the emphasis is to resolve the convective terms accurately.

2.3.1 Physical System

Physical system consists of a 2D channel formed by placing two infinite plates parallel to each other separated by a unit distance, as shown in Fig. 2.4. Flow is assumed to be fully developed at the inlet and gradients along the downstream directions are set to zero for velocity and pressure at the outlet. No-slip boundary conditions are imposed at the top and bottom wall for velocity and the normal pressure gradients are set to zero.

Channel length is represented as L and width is represented as W. The flow Reynolds number is set to 100 and a transient solution technique is adopted.



Fig. 2.4: 2D Channel flow

The flow is assumed to be time dependant and incompressible. Body forces are assumed

to be absent and fluid properties like density and viscosity are taken to be constants.

Boundary Conditions

A fully developed flow profile is fixed at the inlet and no-slip boundary condition is applied at the walls. Streamwise gradients are set to zero for the velocity boundary conditions at the outlet. For pressure, the gradients normal to surfaces are set to zero at the four boundaries. The boundary conditions can be given in the mathematical format as shown below: At top and bottom wall:

$$u = 0,$$
 $v = 0,$ $\frac{\partial p}{\partial y} = 0$

At the left wall (inlet):

$$u = 1 - y^2,$$
 $v = 0,$ $\frac{\partial p}{\partial x} = 0$

At the right wall (outlet):

$$\frac{\partial u}{\partial x} = 0, \qquad \frac{\partial v}{\partial x} = 0, \qquad \frac{\partial p}{\partial x} = 0$$

2.3.2 Results

Channel flow problem was solved for a Re = 100 and the velocity vectors were plotted to visualize the flow profile at subsequent downstream positions as shown in Fig. 2.5.

The velocity vectors are in correspondence to our expectations and analytical solutions. Thus in conclusion this problem validates passive transport handling capacity of our code and we further move on to consider additional complications.



Fig. 2.5: Velocity vectors

2.4 Lid-driven Square Cavity

This is a classic problem for realizing internal recirculating flows within a bounded domain and display several critical fluid flow phenomena in a relatively simplistic geometrical setting. The physical model represents a square cavity with a driven lid on top to induce the recirculation.

2.4.1 Physical System

A square cavity with lid on its top surface is considered as the physical model, as shown in Fig. 2.6. The lid is assigned a horizontal velocity based on profile that remains consistent with zero velocity at the extreme points. No-slip boundary condition is applied at three remaining boundaries. Gradients of pressure normal to the boundaries are set to zero with a special treatment considered later.

The cavity length is defined as L while the height is specified as W. Non-dimensional form of Navier-Stokes equation is used for this problem and so fluid properties have been included in the Reynolds Number. Change in Reynolds number would reflect different working fluids.

Flow is assumed to be incompressible and a transient analysis is carried out. Body forces



Fig. 2.6: Lid-driven cavity

have been neglected and it is valid to assume the characteristic length as the lid dimension. Characteristic velocity is taken to be the average velocity over the lid.

Boundary Conditions

Lid is driven at a velocity which varies along its length and is zero at the boundaries so as to be conformal. Rest of the boundaries are supplied with no-slip conditions.

We had an interesting observation for the pressure boundary conditions which involve gradients at each side. Incompressible flows deal with the gradients of pressure at every stage and the values of pressure themselves do not have any role here. Even in this problem we have a poisson equation governing pressure and the boundary conditions work with gradients. But, in solving the equations numerically pressure becomes unconstrained and it is thereby advised to set the pressure as zero at a point in the computational domain. We have set the pressure to be zero at the square's center.

At left and right wall:

$$u = 0,$$
 $v = 0,$ $\frac{\partial p}{\partial x} = 0$

At the bottom wall:

$$u = 0,$$
 $v = 0,$ $\frac{\partial p}{\partial y} = 0$

At the lid:

$$u = 16x^2(1 - x^2),$$
 $v = 0,$ $\frac{\partial p}{\partial y} = 0$

At the domain's center point:

p = 0

2.4.2 Results and Validation

The computations have been carried out at a range of Reynolds number starting from 100 to 2000. Additional definitions of streamfunction and vorticity are introduced in post processing to examine the streamlines and for quantitative validation.

Vorticity is computed at each time step using,

$$\omega^{n+1} = \frac{\partial v^{n+1}}{\partial x} - \frac{\partial u^{n+1}}{\partial y}$$

The streamfunction ψ is computed using the Poisson equation,

$$\nabla^2 \psi^{n+1} = -\omega^{n+1} \quad in \quad \Omega$$
$$\psi^{n+1} = 0 \quad on \quad \partial \Omega$$

The results were qualitatively validated by comparing the streamfunction contours and the center-line velocity profiles with previous work by Martinez et al, as shown in Fig. 2.7, Fig. 2.8 and Fig. 2.9. N represents elements in the x-direction and M represents y-direction elements. A mesh of 33×33 has been used with a time step of 10^{-3} to guarantee high precision of the results and stability of the method. The Chebyshev-Gauss-Lobatto grid points are beneficial in this probelm due to their condensed distribution at the corners which helps in refining the secondary vortices appropriately.

Convergence is assessed by considering the flow at two values of Re = 100 and 400. Comparisons of some characteristic flow variables are made with those of Botella [8] who used a third order accurate Chebyshev projection scheme, and Ehrenstein and Peyret [18], who used a vorticity-stream function formulation based on Chebyshev collocation method. The comparisons are carried out for different spatial resolutions on the maximal value of streamfunction $|\psi|$ on the inner collocation points and the maximum vorticity value $|\omega|$ on the moving lid.

$M_1 = \max \psi(x_i, y_i) $	on the inner collocation points
$M_2 = \max \omega(x_i, 1) $	on the collocation points of the lid $y = 1$

Table 2.1: Comparison of flow variable M_1 for the square driven cavity at Re = 100.

N = M	M_1	M_1	% Difference
	Present	Botella	Botella
	Method	(1997)	(1997)
17	8.3096E-02	8.3160E-02	0.0770
21	8.2656E-02	8.2694E-02	0.0460
25	8.3285 E-02	8.3315E-02	0.0360
33	8.3381E-02	8.3402 E-02	0.0252

Table 2.2: Comparison of flow variable M_2 for the square driven cavity at Re = 100.

N = M	M_2	M_2	M_2	% Difference	% Difference
	Present	Botella	Ehrenstein &	Botella	Ehrenstein &
	Method	(1997)	Peyret(1989)	(1997)	$\operatorname{Peyret}(1989)$
17	13.3358	13.3467	13.3687	0.0877	0.2521
21	13.1845	13.1759	13.1780	0.0615	0.0455
25	13.4273	13.4226	13.4227	0.0328	0.0320
33	13.3431	13.3423	13.3422	0.0052	0.0060

Tables 2.1 to 2.4, display the comparison of the characteristic flow variables with benchmark solutions prevalent in literature. For Re = 100, the relative errors as shown in Table 2.1 for M_1 and Table 2.2 for M_2 are less than 0.3% when compared with results obtained by Botella [8] and by Ehrenstein and Peyret [18] for a grid of N = M > 17. But for Re = 400, a grid of N = M > 21 gives relative errors in M_1 and M_2 less than 0.2% when compared with the same standards, as shown in Table 2.3 and Table 2.4.

N = M	M_1	M_1	% Difference
	Present	Botella	Botella
	Method	(1997)	(1997)
17	8.5335E-02	8.5777E-02	0.5153
21	8.5107E-02	8.5192 E-02	0.0998
25	8.5664 E-02	8.5716E-02	0.0607
33	8.5461 E-02	8.5480E-02	0.0222

Table 2.3: Comparison of flow variable M_1 for the square driven cavity at Re = 400.

Table 2.4: Comparison of flow variable M_2 for the square driven cavity at Re = 400.

N = M	M_2	M_2	M_2	% Difference	% Difference
	Present	Botella	Ehrenstein &	Botella	Ehrenstein &
	Method	(1997)	Peyret(1989)	(1997)	Peyret(1989)
17	24.7258	24.7799	25.2329	0.2216	2.0128
21	24.6237	24.6268	24.6693	0.0154	0.1877
25	24.9212	24.9157	24.9344	0.0213	0.0537
33	24.7873	24.7845	24.7845	0.0101	0.0101

On observing the relative errors in variables we conclude that for N = M = 33 we get accurate results without compromising the computational speed and thus all the qualitative results have been calculated based on that grid count.

Our results are in good agreement with the benchmark solutions both qualitatively and quantitatively as shown by the plots and tables. Thus in conclusion we have the assurance that the code is able to handle bounded fluid flow problems efficiently.



Fig. 2.7: Steady state streamlines comparison for Re = 100, 400



Fig. 2.8: Steady state streamlines comparison for Re = 1000, 2000



Fig. 2.9: Variation of velocity along the center-line of the driven cavity for different Re

2.5 Natural Convection

Natural convection in a square cavity is considered here at different Rayleigh numbers and compared with existing benchmark solutions. This study will help in validating our code for heat transfer applications and is in a way an extension of the lid-driven problem.

2.5.1 Physical System

Physical system consists of a square cavity which has two opposite sides adiabatic and the other two at two distinct temperatures. The left wall is kept at a temperature T_h and the right wall is kept at a temperature T_c . The cavity length is specified by L and the height of the cavity is defined as H, as shown in Fig. 2.10. Adiabatic wall condition is applied at the top and bottom of the domain.



Fig. 2.10: Natural convection in a square cavity

Natural convection is assumed to be transient and incompressible in nature. Buoyancy

force caused by density variation is taken into account using the Boussinesq approximation. The thermophysical properties are assumed to be invariant with temperature and the body forces are neglected.

Boundary Conditions

No-slip boundary conditions are applied at the walls. Pressure gradients normal to the boundary surfaces are set to zero and additionally pressure at the center of domain is set to zero. The left and right walls are set to constant high and low temperature respectively. The other walls are treated as adiabatic and the boundary conditions are expressed as follows, At the left wall:

$$u = 0,$$
 $v = 0,$ $\frac{\partial p}{\partial x} = 0,$ $T = 1$

At the right wall:

$$u = 0,$$
 $v = 0,$ $\frac{\partial p}{\partial x} = 0,$ $T = 0$

Top wall and bottom wall:

$$u = 0,$$
 $v = 0,$ $\frac{\partial p}{\partial y} = 0,$ $\frac{\partial T}{\partial y} = 0$

At the domain's center:

p = 0

2.5.2 Results

The streamfunction and Temperature contours are plotted for this problem and qualitatively compared with standard benchmark results, as shown in Fig. 2.11.

We can conclude by observing the concurrency of our results with prevalent benchmark solutions that our scheme and code works in solving bounded heat transfer problems. Natural convection in a square cavity serves as a fundamental test case for such prepositions.



Fig. 2.11: Comparison of streamfunction contours [a,b] and isotherms [c,d] for $Ra = 10^7$

2.6 Heat Conduction: Triangular Domain

Spectral methods have a main limitation of being used specifically for regular computational domains and offer challenges when extended to non-regular ones. In this problem we attempt to solve a heat conduction problem for a triangular domain with constant but distinct temperature at the boundaries.

2.6.1 Physical System

The physical model consists of a triangular plate with sides maintained at constant but different temperatures. A right angled triangular plate is considered as our physical system with an orientation conformal to our mapping. Plate length is specified as L and the width is specified as W, as shown in Fig. 2.12. Moreover the present case considers a right-angled isosceles triangle. The solution approach here is to map the coordinates and derivatives from the rectangle to triangular domain.

There is a singularity in the transformation where all the derivatives do not exist and this needs to be tackled appropriately to get physically realistic solutions.



Fig. 2.12: Heat conduction in a triangular plate

Boundary Conditions

At the side wall:

$$T_1 = 500 K$$

At the top wall:

$$T_2 = 400 K$$

At the hypotenuse:

$$T_3 = 300 \, K$$

The domain is discretized using Chebyshev Gauss-Lobatto grid points and derivative

matrices are obtained by expressing the solution in terms of Chebyshev polynomials. A grid size of 30×30 is used in the analysis and is found to be sufficient considering the high accuracy and global nature of spectral methods. The horizontal side at y = -1 in the computational domain is the source of singularity in the derivatives and so we tackled this issue by assigning all the values at this y-level in the derivative matrices to zero.

2.6.2 Results

The isotherms were plotted for this problem and compared with a heat conduction problem solution from the commercial solver ANSYS, as shown in Fig. 2.13. Contours are compared and so this is a qualitative test but is rendered sufficient for bolstering credibility.



Fig. 2.13: Isotherms for the triangular plate

The ANSYS model had roughly 20,000 elements and the upper and right side walls were partitioned into 200 equal sections. The left wall was divided into 283 elements so as to maintain equal element length across the boundaries. Finally, a global element sizing of 5×10^{-3} was enforced to get sufficient refinement near the center of the domain.

Through this problem we can conclude that simple diffusive terms can be handled properly.

Chapter 3

Parallelization of FDM Codes

3.1 1D Heat Conduction

Here we consider 1D heat conduction and use different methods to solve the same numerically. For static heat conduction,

$$\frac{\partial^2 T}{\partial x^2} = S \tag{3.1}$$

We will discuss some methods to solve 1D-conduction problems with varying number of points using different methods. We have considered the physical system depicted in fig. 3.1 with boundary conditions as $T_{\text{left}} = 300 \text{ K}$ and $T_{\text{right}} = 400 \text{ K}$



Fig. 3.1: 1D Heat conduction

Equation 3.1 is discretized using finite difference method to obtain a system of linear equations, solution of which gives the temperature distribution along the discrete points considered.

$$a_i T_i = b_i T_{i+1} + c_i T_{i-1} + d_i \quad \text{where } i = 1, 2, 3, \dots, N$$

$$(3.2)$$

To account for the boundary points,

$$c_1 = 0 \quad and \quad b_N = 0 \tag{3.3}$$

3.1.1 Jacobi Iterative Method

Jacobi method is an iterative method to solve a system of linear equations (Ax = b) which starts with some initial guess. The result x at an iteration k is evaluated using the following approach,

$$\sigma_i = \sum_{j=1, \ j \neq i}^n a_{ij} x_j^{(k)} \quad \text{where } i = 1, 2, 3, \dots, N$$
(3.4)

$$x_i^{(k+1)} = \frac{1}{a_{ii}} (b_i - \sigma_i) \quad \text{where } i = 1, 2, 3, \dots, N$$
(3.5)

For the purpose of parallelization we have computed for different x_i in parallel during each iteration. Each processor is assigned a block of rows (x_i) dynamically using the !\$OMP DO SCHEDULE(dynamic, [chunk size]) constuct.

No. of points	Serial execution	Parallel	Observed
	Clock time (s)	execution Clock	speed-up
		time (s)	
100	0.7445	0.2052	3.6281
200	10.4809	2.7152	3.8601

 Table 3.1:
 Jacobi iterative method

The table 3.1 shows that the observed speed - up of the parallel code against the serial code is around 3.6 to 3.8. We used a quad - core CPU so the ideal speed-up is limited to 4.

3.1.2 Domain Decomposition in Space

In spatial domain decomposition method the physical domain is divided into a number of sub-domains. We will use Tri-Diagonal Matrix Algorithm (TDMA) to solve each sub-domain individually. In parallel version each domain is solved by a different core. Initially we implemented for two sub-domains which was later extended to N domains. An initial guess



Fig. 3.2: Temperature distribution using Jacobi method

is made for the interface temperature and heat flux which serves as the boundary conditions for the sub-domains. We then solve the two sub-domains in an iterative process. At the interface of two sub-domains,

$$T_{\rm i, \, left} = \frac{T_{\rm i, \, left} + T_{\rm i, \, right}}{2} \tag{3.6}$$

$$Q_{\rm i, \ right} = \frac{Q_{\rm i, \ left} + Q_{\rm i, \ right}}{2} \tag{3.7}$$

We use the following termination conditions,

$$|Q_{i, left} - Q_{i, right}| < \epsilon_1 \quad and \quad |T_{i, left} - T_{i, right}| < \epsilon_2$$
(3.8)

No. of points	Iterations	Serial	Parallel	Observed
	required	execution	execution	speed-up
		Clock time (s)	Clock time (s)	
1000	32	4.65616E-3	2.53811E-3	1.8345
2000	35	1.11364E-2	5.97120E-3	1.8650

 Table 3.2: Domain decomposition with two subdomains

Table 3.2 shows the results for domain decomposition using two sub-domains. We can

No. of points	Iterations	Serial	Parallel	Observed
	required	execution	execution	speed-up
		Clock time (s)	Clock time (s)	
1000	153	9.22481E-3	2.82501E-3	3.2654
2000	158	1.74712E-2	5.10879E-3	3.4112

see that the observed speed-up is close 2. Here we are restricted to use only two cores for the parallel code as we are limiting to use only two sub-domains.

 Table 3.3: Domain decomposition with four subdomains

Table 3.3 shows the results for domain decomposition using four sub-domains. Though we can see a speed-up of about 3.2 to 3.4 however, the execution time for the serial code with four sub-domains is actually more than that for two sub-domains (comparing to results of table 3.2). The execution time for parallel version of code with four sub-domains is slightly less than that for two sub-domains. We can also notice that the number iterations required have increased. This can be explained by looking at how the information travels from the left end to the right end. With four sub-domains we have three interfaces which obstruct the flow of information in a single go. But as we solve the sub-domains parallely the execution time is slightly less.

This may give a notion that domain decomposition isn't a useful method. But we should note that we have taken the initial guess at interface as random, which can be improved if we first use a coarse mesh to get initial guesses.

In this chapter we provided details of the Jacobi iterative method and Domain decomposition method which we have used to solve the 1D heat conduction problems using parallel computing. We can see that the domain decomposition method using TDMA is much faster than Jacobi iterative method. We also saw that for domain decomposition method as the number of sub-domains increased the execution time increased as our initial guesses were random.



Fig. 3.3: Temperature distribution using domain decomposition

3.2 2D Heat Conduction

Here we consider 2D heat conduction and use different numerical methods to solve the same with varying grid size. For a 2-D domain with uniform conductivity, the static heat conduction equation,

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = S \tag{3.9}$$

We have considered the physical system depicted in fig. 3.4 with boundary conditions as $T_{\text{bottom}} = 300 \text{ K}$ and T = 400 K on other three sides. Equation 3.9 is discretized using finite difference method to obtain a system of linear equations, solution of which gives the temperature distribution along the discrete points considered.

Using finite difference discretization,

$$2(1+h^2)T_P = T_{\text{East}} + T_{\text{West}} + h^2(T_{\text{North}} + T_{\text{South}}) - S\Delta x^2$$
(3.10)

where,
$$h = \frac{\Delta x}{\Delta y}$$



Fig. 3.4: 2D Heat conduction

3.2.1 TDMA Sweeps

TDMA Sweeps is line-by-line method to solve 2-D and 3-D systems which combines Gauss-Seidel and TDMA methods. The grid points along a line are solved iteratively using TDMA. The other terms are treated as constant for solving the grid points along the chosen line as shown in fig. 3.5.



Fig. 3.5: TDMA line-by-line method [Patankar [1]]

The region is sweeped line-by-line in two directions using TDMA alternatively, first in

horizontal direction then in vertical direction. We have used the following condition for termination incorporating l_2 norm given as,

$$||X - X_{\text{prev}}||_2 < \epsilon \tag{3.11}$$

Grid size	Serial execution	Parallel	Observed
	Clock time (s)	execution Clock	speed-up
		time (s)	
100 x 100	1.4427	0.6469	2.230
$200 \ge 200$	19.9946	8.4437	2.368

 Table 3.4:
 TDMA sweeps method

Table 3.4 shows the results for TDMA sweeps for 2-D heat conduction. The observed speed - up is around 2.3 even though we used four processors. This could be due to the overhead of calculating the norm of $X - X_{prev}$ at each iteration.



Fig. 3.6: Temperature distribution using TDMA sweeps

3.2.2 Domain Decomposition with Two Sub-Domains

Similar to 1-D domain decomposition the domain is divided into multiple sub-domains, the only difference being the sub-domains are rectangular. TDMA sweeps has been used to solve each rectangular sub-domain. Similar to 1D domain decoposition each domain is solved by a different core concurrently in the parallel version of the code. For now it has been implemented for two subdomains which will be extended to N domains later. At the interface of two sub-domains,

$$T_{iNx_1, left} = \frac{T_{iNx_1, left} + T_{i1, right}}{2} \quad \text{where } i = 1, 2, \dots, N_y \tag{3.12}$$

$$Q_{i1,right} = \frac{Q_{iNx_1,left} + Q_{i1,right}}{2} \quad \text{where } i = 1, 2, \dots, N_y \tag{3.13}$$

Grid size	Iterations	Serial	Parallel	Observed
	required	execution	execution	speed-up
		Clock time	Clock time	
		(s)	(s)	
100 x 100	5	7.74840	5.03571	1.5386
$200\ge 200$	6	98.70741	62.33654	1.5835

 Table 3.5:
 2D domain decomposition with two sub-domains

Table 3.5 shows the results for 2-D domain decomposition using two sub-domains. Though we can see a speed-up of about 1.5 to 1.6 however, the execution time for code with two sub-domains is actually more than that for TDMA Sweeps (comparing to results of table 3.4). It should also be noted that the number of iterations of TDMA sweeps for domain decomposition is 5-6 whereas if we use TDMA sweeps alone only one iteration of TDMA sweeps is required.

This can explained by looking at how the information travels from left end to the right end in domain decomposition. Similar to 1-D the interface of two sub-domains obstructs the flow of information in a single go. As in 1-D the initial guess for temperature and heat flux is taken to be random which can be improved by using results of coarse mesh as initial guess.



Fig. 3.7: Temperature distribution using domain decomposition

TDMA sweeps was found to be better as with domain decomposition method the interface obstructs the flow of information. While using a uniform mesh we find TDMA sweeps to be of more use however, to solve non-uniform mesh domain decomposition will be greater use. Domain decomposition can further be improved by using coarse mesh to get the initial guesses.

Chapter 4

Parallelization of Spectral Codes

Spectral methods use a predefined Chebyshev grid for the given number of elements and computational domain. The Chebyshev grid is characteristically fine at the corners but relatively coarser in the mid-section of the domain. As a result, in problems involving resolution of flow phenomena near the center of the domain we must resort to higher number of elements. Moreover, spectral methods exhibit consistent accuracy above a threshold grid size implying that further refinements would increase computations without improving accuracy. Thus partitioning the domain and solving each of them using spectral method would result in refinements within the domain.

4.1 One Dimensional Heat Conduction

In this section we solve the simplest problem of one-dimensional heat conduction to develop the framework for domain decomposition in spectral methods.

4.1.1 Physical System

The physical model can be thought to be a slender rod with sides maintained at constant but different temperatures. This slender assumption retains the one-dimensional nature of the problem. Rod length is specified as L as shown in Fig. 4.1. Moreover, the width is neglected in comparison to length of the rod giving a one-dimensional domain.



Fig. 4.1: 1D Heat conduction

Boundary Conditions

At the left side:

$$T_1 = 100 K$$

At the right side:

$$T_2 = 0 K$$

At the left side of interface:

$$T = T_{i,left}$$

At the right side of interface:

$$\frac{\partial T}{\partial x} = -q_{\rm i, right}$$

The domain is discretized using Chebyshev Gauss-Lobatto grid points and derivative matrices are obtained by expressing the solution in terms of Chebyshev polynomials. The boundary conditions at the interface are updated at each iteration using the following formulation:

$$T_{\text{inter}} = \frac{T_{\text{i,left}} + T_{\text{i,right}}}{2}$$
$$q_{\text{inter}} = \frac{q_{\text{i,left}} + q_{\text{i,right}}}{2}$$

Boundary conditions at the interface are then updated to T_{inter} and q_{inter} for the next iteration, that is T_{inter} is assigned to $T_{\text{i,left}}$ and q_{inter} is assigned to $q_{\text{i,right}}$.

4.1.2 Results

The iterative method is carried out until the errors at interface are reduced to the order below 10^{-6} . Two errors are defined corresponding to temperature and heat flux values at the two sides of the interface and are based on the maximum difference of values at the interface.

$$\operatorname{error}_{\mathrm{T}} = \max(\operatorname{abs}(T_{\mathrm{i,left}} - T_{\mathrm{i,right}}))$$

$$\operatorname{error}_{q} = \max(\operatorname{abs}(q_{i,\text{left}} - q_{i,\text{right}}))$$

Serial and parallel run times were noted for five runs of the code based on different grid sizes. The speed up was calculated for each case and was observed to be in accordance with expectations ranging from 1.16 to 1.51. Speed up improved with refinements in grid which is expected as significant computational load is effectively split between the processors exhibiting a time advantage. Table 4.1 summarizes the results.

 Table 4.1: Comparison of serial, parallel times and speed-up over various grid sizes for 1D conduction.

Number of grid	Serial Execution	Parallel Execution	Observed
points (per	Clock Time (s)	Clock Time (s)	Speed-Up
$\operatorname{subdomain})$			
30	0.198	0.171	1.16
40	0.358	0.280	1.28
50	0.570	0.432	1.32
60	0.838	0.574	1.46
70	1.174	0.785	1.51

4.2 Two Dimensional Heat Conduction

4.2.1 Domain Decomposition with Two Subdomains

In this problem we extend our knowledge of domain decomposition in one-dimensional problems to two-dimensional ones. This section deals with dividing the domain into two parts and solving them individually using spectral method.

Physical System

The physical model consists of a rectangular plate with sides maintained at constant but different temperatures. A partition is made at the center of the plate in the computational domain but the final solution is reflected as a whole.

Plate length is specified as L and the width is specified as W, as shown in Fig. 4.2. Moreover the partition is made at length 0.5L giving us two sub-domains each of length 0.5Land width W.



Fig. 4.2: 2D Heat conduction - two subdomains

Boundary Conditions

At the top wall:

$$T_h = 400 \, K$$
At the left, right and bottom wall:

$$T_c = 300 \, K$$

At the left side of interface:

$$T = T_{i,left}$$

At the right side of interface:

$$\frac{\partial T}{\partial x} = -q_{\rm i, right}$$

The domain is discretized using Chebyshev Gauss-Lobatto grid points and derivative matrices are obtained by expressing the solution in terms of Chebyshev polynomials. Similar to the one-dimensional case, boundary conditions at the interface are updated at each iteration using the following formulation:

$$T_{\text{inter}} = \frac{T_{\text{i,left}} + T_{\text{i,right}}}{2}$$
$$q_{\text{inter}} = \frac{q_{\text{i,left}} + q_{\text{i,right}}}{2}$$

Boundary conditions at the interface are then updated to T_{inter} and q_{inter} for the next iteration, that is T_{inter} is assigned to $T_{\text{i,left}}$ and q_{inter} is assigned to $q_{\text{i,right}}$.

Results

The iterative method is carried out until the errors at interface are reduced to the order below 10^{-6} . Two errors are defined corresponding to temperature and heat flux values at the two sides of the interface and are based on the maximum difference of values at the interface.

$$\operatorname{error}_{\mathrm{T}} = \max(\operatorname{abs}(T_{\mathrm{i,left}} - T_{\mathrm{i,right}}))$$

$$\operatorname{error}_{q} = \max(\operatorname{abs}(q_{i,\text{left}} - q_{i,\text{right}}))$$

Comparing the numerical solution with analytical result we observe that they coincide exactly thereby verifying spectral accuracy. Also, refinements near the center can be observed in plot 4.3 with concentrated points at the corners and center.



Fig. 4.3: Midline profile comparison

Solutions from both the domains were combined finally to constitute an overall temperature field. Thereafter, a temperature contour plot shown in Fig 4.4 helped in assuring continuity among the results from the left and right sub-domains.

Serial and parallel run times were noted for five runs of the code based on different grid sizes. The speed up was calculated for each case and was observed to be in accordance with expectations ranging from 1.38 to 1.89. Speed up improved with refinements in grid which is expected as significant computational load is effectively split between the processors exhibiting a time advantage. Table 4.2 summarizes the results.



Fig. 4.4: Temperature contour plot for two subdomains

Table 4.2: Comparison of serial, parallel times and speed-up over various grid sizes for 2D conduction with two subdomains.

Number of grid	Serial Execution	Parallel Execution	Observed
points (per	Clock Time (s)	Clock Time (s)	Speed-Up
$\operatorname{subdomain})$			
20×20	1.027	0.746	1.38
30×30	9.693	5.584	1.74
35×35	23.635	12.910	1.83
40×40	51.222	27.329	1.88
50×50	190.84	101.24	1.89

4.2.2 Domain Decomposition with Four Subdomains

This section extends over the previous case and deals with dividing the domain into four parts, solving them individually. This formulation serves crucial for extending the algorithm to domain decomposition involving multiple sub-domains.

Physical System

The physical model consists of a rectangular plate with sides maintained at constant but different temperatures. Partition are made at the center of the plate in the computational domain but the final solution is reflected as a whole.

Plate length is specified as L and the width is specified as W, as shown in Fig. 4.5. Moreover partitions are made at length 0.5L and width 0.5L, giving us four sub-domains each of length 0.5L and width 0.5W.



Fig. 4.5: 2D Heat conduction - four subdomains

Boundary Conditions

At the top wall:

$$T_h = 400 \, K$$

At the left, right and bottom wall:

$$T_c = 300 \, K$$

Interface boundary conditions are critical for this problem because it was observed that

having two Neumann boundary conditions in a domain leads to divergence. These boundary conditions are initially random guesses which are updated every iteration to finally give a physically realistic result. So the interface conditions follow the pattern given in fig 4.5

The domain is discretized using Chebyshev Gauss-Lobatto grid points and derivative matrices are obtained by expressing the solution in terms of Chebyshev polynomials. Similar to the one-dimensional case, boundary conditions at the interface are updated at each iteration using the following formulation:

$$T_{\text{inter}} = \frac{T_{\text{i,left}} + T_{\text{i,right}}}{2}$$
$$q_{\text{inter}} = \frac{q_{\text{i,left}} + q_{\text{i,right}}}{2}$$

Boundary conditions at the interface are then updated to T_{inter} and q_{inter} for the next iteration, that is T_{inter} is assigned to $T_{\text{i,left}}$ and q_{inter} is assigned to $q_{\text{i,right}}$.

Results

The iterative method is carried out until the errors at interface are reduced to the order below 10^{-6} . Two errors are defined corresponding to temperature and heat flux values at the two sides of the interface and are based on the maximum difference of values at the interface.

$$\operatorname{error}_{\mathrm{T}} = \max(\operatorname{abs}(T_{\mathrm{i,left}} - T_{\mathrm{i,right}}))$$

$$\operatorname{error}_{q} = \max(\operatorname{abs}(q_{i,\text{left}} - q_{i,\text{right}}))$$

Comparing the numerical solution with analytical result we observe that they coincide exactly thereby verifying spectral accuracy. For this problem we have two mid-lines and the values of temperature are compared along these as shown in Fig. 4.6 and Fig. 4.7. In addition, refinements at the center of the domain can be observed by the clustering of points near the corners and mid-portion of the plots.



Fig. 4.6: Vertical midline profile comparison



Fig. 4.7: Horizontal midline profile comparison

Solutions from all four domains were combined finally to constitute an overall temperature field. Thereafter, a temperature contour plot shown in Fig 4.8 helped in assuring continuity among the results from the four sub-domains together.



Fig. 4.8: Temperature contour plot for four subdomains

Serial and parallel run times were noted for five runs of the code based on different grid sizes. The speed up was calculated for each case and was observed to be in accordance with expectations ranging from 2.43 to 2.71. Speed up improved with refinements in grid which is expected as significant computational load is effectively split between the processors exhibiting a time advantage. Table 4.3 summarizes the results.

Table 4.3: Comparison of serial, parallel times and speed-up over various grid sizes for 2D conduction with four subdomains.

Number of grid	Serial Execution	Parallel Execution	Observed
points (per	Clock Time (s)	Clock Time (s)	Speed-Up
$\operatorname{subdomain})$			
20×20	6.76	2.782	2.43
30×30	54.964	21.811	2.52
35×35	120.47	46.694	2.58
40×40	235.43	89.178	2.64
50×50	746.68	275.528	2.71

4.3 Channel Flow

4.3.1 Domain Decomposition with Two Subdomains

This section extends the algorithm of domain decomposition in spectral methods to fluid flow problems. Previous problems established the method for elliptic equations covered predominantly using heat conduction. Current section deals with a simple problem involving fully developed flow between two parallel plates.

Physical System

The physical model consists of a fully developed flow between two infinite parallel plates separated by a unit distance. Flow is assumed to be fully developed at the inlet and gradients along streamwise directions are set to zero for velocity and pressure at the outlet. The top and bottom walls have a no-slip boundary condition for velocity and zero normal pressure gradients.

Plate length is specified as L and the width is specified as W, as shown in Fig. 4.9. Moreover, a partition is made at length 0.5L, giving us two sub-domains each of length 0.5Land width W. Reynolds number is set to 10 and a transient solution technique is adopted.

Flow is assumed to be incompressible with constant fluid properties and the body forces are assumed to be absent. The grid generated by combining the two domains can be seen as given in Fig. 4.10.

Boundary Conditions

A fully developed flow profile is provided at the inlet and no-slip condition is applied at the walls. Streamwise gradients are set to zero for velocity at the outlet. Pressure gradients normal to the surfaces are set to zero at the four boundaries.

At the interface, nature of boundary condition plays a major role in achieving convergence of the iterative method. We observed that velocity derivatives need to be supplied at the left







Fig. 4.10: Combined grid layout for two subdomains

interface and pressure derivatives at the right interface. At the top and bottom wall:

$$u = 0,$$
 $v = 0,$ $\frac{\partial p}{\partial y} = 0$

At the inlet:

$$u = 1 - y^2, \qquad v = 0, \qquad \frac{\partial p}{\partial x} = 0$$

At the outlet:

$$\frac{\partial u}{\partial x} = 0, \qquad \frac{\partial v}{\partial x} = 0, \qquad \frac{\partial p}{\partial x} = 0$$

At the left interface:

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial x_i}, \qquad \frac{\partial v}{\partial x} = \frac{\partial v}{\partial x_i}, \qquad p = p_i$$

At the right interface:

$$u = u_i, \qquad v = v_i, \qquad \frac{\partial p}{\partial x} = \frac{\partial p}{\partial x_i}$$

Interface values for primitive variables are updated after each iteration in the same way as represented in the conduction problems involving T_i and q_i .

Results

The iterative method is carried out until the errors at interface are reduced to the order below 10^{-6} . Two errors are defined each for u, v velocity components and pressure at the two sides of the interface, similar to temperature and heat flux errors defined in conduction problems.

Solutions from both the domains were combined finally to constitute an overall field for velocity components and pressure. Thereafter, a velocity vector plot given by Fig.4.11 helped in ensuring function continuity at the interface and providing a qualitative idea of solution accuracy.

Serial and parallel run times were noted for five runs of the code based on different grid sizes. The speed up was calculated for each case and was observed to be in accordance with expectations ranging from 1.65 to 1.79. Speed up improved with refinements in grid which is expected as significant computational load is effectively split between the processors exhibiting a time advantage. Table 4.4 summarizes the results.



Fig. 4.11: Velocity vectors for channel flow with two subdomains

Table 4.4: Comparison of serial, parallel times and speed-up over various grid sizes for channel flow with two subdomains.

Number of grid	Serial Execution	Parallel Execution	Observed
points (per	Clock Time (s)	Clock Time (s)	Speed-Up
subdomain)			
10×20	13.555	8.215	1.65
15×30	78.734	46.865	1.68
20×40	271.54	157.87	1.72
30×30	345.53	198.58	1.74
25×50	694.41	387.94	1.79

4.3.2 Domain Decomposition with Four Subdomains

This problem considers a two-dimensional channel flow between infinite parallel plates with four sub-domains. Current formulation serves as a foundation for observing the behaviour of our algorithm in the presence of multiple sub-domains.

Physical System

The physical model consists of a fully developed flow between two infinite parallel plates separated by a unit distance. Flow is assumed to be fully developed at the inlet and gradients along streamwise directions are set to zero for velocity and pressure at the outlet. The top and bottom walls have a no-slip boundary condition for velocity and zero normal pressure gradients.

Plate length is specified as L and the width is specified as W, as shown in Fig. 4.12. Moreover, partitions are made at length 0.5L and width 0.5W, giving us four sub-domains each of length 0.5L and width 0.5W. Reynolds number is set to 10 and a transient solution technique is adopted.

Flow is assumed to be incompressible with constant fluid properties and the body forces are assumed to be absent. Only derivatives are represented using $D_{u,v}$ and D_p in Fig. 4.12 to preserve clarity and other interface boundary conditions should be taken as value assignment type. The grid generated by combining the four domains can be seen as given in Fig. 4.13.



Fig. 4.12: Channel flow - four subdomains



Fig. 4.13: Combined grid layout for four subdomains

Boundary Conditions

A fully developed flow profile is provided at the inlet and no-slip condition is applied at the walls. Streamwise gradients are set to zero for velocity at the outlet. Pressure gradients normal to the surfaces are set to zero at the four boundaries.

Building upon the previous problem, the interface boundary conditions play a cardinal role in obtaining a correct solution. Fig. 4.12 shows the pattern in which boundary conditions should be assigned extending from two subdomains.

At the top and bottom wall:

$$u = 0,$$
 $v = 0,$ $\frac{\partial p}{\partial y} = 0$

At the inlet:

$$u = 1 - y^2,$$
 $v = 0,$ $\frac{\partial p}{\partial x} = 0$

At the outlet:

$$\frac{\partial u}{\partial x} = 0, \qquad \frac{\partial v}{\partial x} = 0, \qquad \frac{\partial p}{\partial x} = 0$$

The interface boundary conditions are shown in Fig. 4.12. Interface values for primitive variables are updated after each iteration in the same way as represented in the conduction problems involving T_i and q_i .

Results

The iterative method is carried out until the errors at interface are reduced to the order below 10^{-6} . Two errors are defined each for u, v velocity components and pressure at the two sides of the interface, similar to temperature and heat flux errors defined in conduction problems.

Solutions from all four domains were combined finally to constitute an overall field for velocity components and pressure. Thereafter, a velocity vector plot given by Fig.4.14 helped in ensuring function continuity at the interface and providing a qualitative idea of solution accuracy.

Serial and parallel run times were noted for five runs of the code based on different grid sizes. The speed up was calculated for each case and was observed to be in accordance with expectations ranging from 2.36 to 2.83. Speed up improved with refinements in grid which is expected as significant computational load is effectively split between the processors exhibiting a time advantage. Table 4.5 summarizes the results.



Fig. 4.14: Velocity vectors for channel flow with four subdomains

Table 4.5: Comparison of serial, parallel times and speed-up over various grid sizes forchannel flow with four subdomains.

Number of grid	Serial Execution	Parallel Execution	Observed
points (per	Clock Time (s)	Clock Time (s)	Speed-Up
subdomain)			
10×10	13.197	5.5919	2.36
15×15	79.347	31.487	2.52
20×20	255.39	96.739	2.64
25×25	664.85	241.76	2.75
30×30	1438.6	508.34	2.83

4.4 Lid Driven Cavity

4.4.1 Domain Decomposition with Two Subdomains

This section considers a slightly advanced fluid flow problem for realizing internal recirculating flows within a bounded domain. The model physically represents a square cavity with a driven lid to induce recirculation. Computational space is divided into two subdomains, each of which is solved using spectral method exchanging information at the interface.

Physical System

A square enclosure with driven lid on its top surface is taken as the physical model, as shown in Fig. 4.15. No-slip boundary condition is applied at the walls barring the lid which is driven with a profile consistent with zero velocity at the edges. Normal to the surface pressure gradients are set to zero.

Enclosure length is specified as L and the width is specified as W, as shown in Fig. 4.15. Moreover, a partition is made at length 0.5L, giving us two sub-domains each of length 0.5Land width W.

Flow is assumed to be incompressible with constant fluid properties and the body forces are assumed to be absent.

Boundary Conditions

No-slip boundary condition is enforced over all the walls except the lid which is driven at a velocity conformal to zero value at the edges. Pressure gradients normal to the boundary surfaces are set to zero and in addition pressure value at the center of the cavity is taken to be zero.

Building upon the previous problem, the interface boundary conditions play a cardinal role in obtaining a correct solution. The resulting boundary conditions can be mathematically given as,



Fig. 4.15: Lid driven cavity - two subdomains

At the left and right wall:

$$u = 0,$$
 $v = 0,$ $\frac{\partial p}{\partial x} = 0$

At the bottom wall:

$$u = 0,$$
 $v = 0,$ $\frac{\partial p}{\partial y} = 0$

At the lid:

$$u = 16x^2(1 - x^2),$$
 $v = 0,$ $\frac{\partial p}{\partial y} = 0$

At the domain's center point:

$$p = 0$$

At the left interface:

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial x_i}, \qquad \frac{\partial v}{\partial x} = \frac{\partial v}{\partial x_i}, \qquad p = p_i$$

At the right interface:

$$u = u_i, \qquad v = v_i, \qquad \frac{\partial p}{\partial x} = \frac{\partial p}{\partial x_i}$$

Interface values for primitive variables are updated after each iteration in the same way as represented in the conduction problems involving T_i and q_i .

Results

The iterative method is carried out until the errors at interface are reduced to the order below 10^{-6} . Two errors are defined each for u, v velocity components and pressure at the two sides of the interface, similar to temperature and heat flux errors defined in conduction problems.

Solutions from both the domains were combined finally to constitute an overall field for velocity components and pressure. Thereafter, a velocity vector plot given by Fig.4.16 helped in ensuring function continuity at the interface and providing a qualitative idea of solution accuracy.

Serial and parallel run times were noted for five runs of the code based on different grid sizes. The speed up was calculated for each case and was observed to be in accordance with expectations ranging from 1.78 to 1.91. Speed up improved with refinements in grid which is expected as significant computational load is effectively split between the processors exhibiting a time advantage. Table 4.6 summarizes the results.

Table 4.6: Comparison of serial, parallel times and speed-up over various grid sizes for lid driven cavity with two subdomains.

Number of grid	Serial Execution	Parallel Execution	Observed
points (per	Clock Time (s)	Clock Time (s)	Speed-Up
subdomain)			
10×20	38.855	21.829	1.78
15×30	218.81	120.23	1.82
20×40	730.47	392.73	1.86
30×30	931.45	492.83	1.89
25×50	1858.7	973.14	1.91



Fig. 4.16: Velocity vectors for lid driven flow at Re = 10

4.4.2 Domain Decomposition with Four Subdomains

This section extends the previous problem dividing the computational domain into four subdomains. Each of the subdomains share information at their interfaces and this problem examines the characteristics of our algorithm with multiple subdomains.

Physical System

A square enclosure with driven lid on its top surface is taken as the physical model, as shown in Fig. 4.17. No-slip boundary condition is applied at the walls barring the lid which is driven with a profile consistent with zero velocity at the edges. Normal to the surface pressure gradients are set to zero.

Enclosure length is specified as L and the width is specified as W, as shown in Fig. 4.15. Moreover, partitions are made at length 0.5L and width 0.5W, giving four sub-domains each of length 0.5L and width 0.5W. Flow is assumed to be incompressible with constant fluid properties and the body forces are assumed to be absent.



Fig. 4.17: Lid driven cavity - four subdomains

Boundary Conditions

No-slip boundary condition is enforced over all the walls except the lid which is driven at a velocity conformal to zero value at the edges. Pressure gradients normal to the boundary surfaces are set to zero and in addition pressure value at the center of the cavity is taken to be zero.

Building upon the previous problem, the interface boundary conditions play a cardinal role in obtaining a correct solution. Fig. 4.17 shows the pattern in which boundary conditions should be assigned extending from two subdomains. The resulting boundary conditions can be mathematically given as, At the left and right wall:

$$u = 0,$$
 $v = 0,$ $\frac{\partial p}{\partial x} = 0$

At the bottom wall:

$$u = 0,$$
 $v = 0,$ $\frac{\partial p}{\partial y} = 0$

At the lid:

$$u = 16x^2(1 - x^2),$$
 $v = 0,$ $\frac{\partial p}{\partial y} = 0$

At the domain's center point:

p = 0

The interface boundary conditions are shown in Fig. 4.17. Interface values for primitive variables are updated after each iteration in the same way as represented in the conduction problems involving T_i and q_i .

Results

The iterative method is carried out until the errors at interface are reduced to the order below 10^{-6} . Two errors are defined each for u, v velocity components and pressure at the two sides of the interface, similar to temperature and heat flux errors defined in conduction problems.

Serial and parallel run times were noted for five runs of the code based on different grid sizes. The speed up was calculated for each case and was observed to be in accordance with expectations ranging from 2.57 to 2.87. Speed up improved with refinements in grid which is expected as significant computational load is effectively split between the processors exhibiting a time advantage. Table 4.7 summarizes the results.

Table 4.7: Comparison of serial, parallel times and speed-up over various grid sizes for liddriven cavity with four subdomains.

Number of grid points (per	Serial Execution Clock Time (s)	Parallel Execution Clock Time (s)	Observed Speed-Up
subdomain)			
10×10	33.836	13.924	2.43
15×15	209.54	83.151	2.52
20×20	733.16	284.17	2.58
25×25	1786.4	676.67	2.64
30×30	4020.7	1483.7	2.71

Chapter 5

Conclusions

In this work, CFD solver for the computation of incompressible heat transfer and fluid flows is developed. The solver for incompressible heat transfer and fluid flows is based on spectral method. The parallelization of these codes is based on the domain decomposition method using OpenMP.

For incompressible flows:

- 1. Heat conduction in rectangular domains has been verified with analytical solutions and can be concluded to be coherent with the same.
- 2. Results for the Lid-driven cavity are in strong agreement with benchmarks and the maximum percentage error is found to be less than 2%
- 3. Natural convection results of streamfunction contours and isotherms are found to be matching high-accuracy solutions prevalent in literature.
- 4. Heat conduction in triangular domain has been successfully verified with results from ANSYS and so the code can be asserted as applicable to non-rectangular domains for conduction problems.

In conclusion these problems helped establish our algorithm as general for incompressible fluid flow and heat transfer problems. For parallelization:

- 1. One dimensional and Two dimensional heat conduction codes formulated using FDM were successfully parallelized using two and four subdomains.
- 2. Parallelization of Spectral codes for conduction was carried out using 1D and 2D problems using two and four subdomains with speed up ranging from 1.69 to 2.73.
- Finally the algorithm for domain decomposition was extended to solve fluid flow cases using channel flow and lid driven cavity problems with speed up ranging from 1.74 to 2.91.

In conclusion, the algorithm of domain decomposition for parallelization was deemed to be working for conduction and simple fluid flow problems using both spectral methods and FDM for discretization.

5.1 Future Scope

The present work has the following potential future scope:

- 1. Heat and fluid flow problems can be handled in irregular domains using spectral methods by incorporating appropriate grid transformation techniques.
- 2. Refining the domain decomposition codes for fluid flow problems to attain better speed-up and to solve high Reynolds number situations.
- 3. Extending domain decomposition method to heat flow problems based on the foundations of fluid flow algorithms.
- 4. Handling conduction problems in irregular geometries using the domain decomposition algorithm developed for regular domains and a suitable transformation.

References

- Suhas V. Patankar. Numerical Heat Transfer and Fluid Flow. CRC Press, Taylor & Francis Group, 2009.
- [2] Llyod N. Trefethen. Spectral Methods in Matlab. Society for Industrial and Applied Mathematics (SIAM).
- [3] P. R. Spalart, R. D. Moser and M. M. Rogers. Spectral Methods for the Navier-Stokes Equations with One Infinite and Two Periodic Directions. Journal of Computational Physics, 1991, 297-324.
- [4] C. Canuto, M. Y. Hussaini, A. Quarteroni and T. A. Zang. Spectral Methods in Fluid Dynamics. Springer-Verlag, Berlin, 1987.
- [5] D. Gottlieb and S. A. Orszag. Numerical Analysis of Spectral Methods. SIAM, Philadelphia, 1977.
- [6] A. Solomonoff and E. Turkel. Global Properties of Pseudospectral Methods. Computational Physics, Vol. 81, 1989, 239-276.
- [7] M. Deville, P. F. Fischer and E. H. Mund. High-Order Methods for Incompressible Fluid Flow. Cambridge Monographs on Applied and Computational Mathematics. Cambridge University Press, 2002.
- [8] O. Botella. On the Solution of Navier-Stokes Equations using Chebyshev Projection Schemes with Third-Order accuracy in Time. Computers & Fluids, Vol. 26, 1997, 107-116.

- [9] A. J. Chorin. Numerical Solution of the Navier-Stokes Equations. Mathematics of Computation, Vol. 22, 1968, 745-762.
- [10] R. Temam. Une Mthode dApproximation de la Solution des quations de Navier-Stokes.
 Bulletin of Society Mathematics of France, Vol. 98, 1968, 115-152.
- [11] S. Huges and A. Randriamampianina. An Improved Projection Scheme Applied to Pseudospectral Methods for the Incompressible Navier-Stokes Equations. International Journal for Numerical Methods in Fluids, Vol. 28, 1998, 501-521.
- [12] C. L. Streett and M. G. Macaraeg. Spectral Multi-Domain for Large-Scale Fluid Dynamic Simulations. Applied Numerical Mathematics, Vol. 6, 1989/90, 123-139.
- [13] William D. Gropp and David E. Keyes. Domain Decomposition Methods In Computational Fluid Dynamics. International Journal For Numerical Methods In Fluids, Vol. 14, 147-165, 1992.
- [14] L.M.R. Carvalho and J.M.L.M. Palma. Parallelization of CFD Code Using PVM and Domain Decomposition Techniques. International Conference on Vector and Parallel Processing, 247-257, 1996.
- [15] Maria Giuseppina Chiara Nestola, Barna Becsekb, Hadi Zolfagharib, Patrick Zuliana, Dario De Marinisb, Rolf Krausea and Dominik Obristb. An immersed boundary method for fluid-structure interaction based on overlapping domain decomposition. Journal of Computational Physics, 2018.
- [16] A. Jagannathan, R. Mohan and M. Dhanak. A spectral method for the triangular cavity flow. Computers & Fluids, Vol. 95, 2014, 40-48.
- [17] J. P. Holman. *Heat Transfer*. Mc-Graw Hill Higher Education, 1977.

- [18] U. Ehrenstein and R. Peyret A Chebyshev Spectral Collocation Method for the Navier-Stokes Equations with Application to Double-Diffusive Convection. International Journal for Numerical Methods in Fluids, Vol. 9, 1989, 427-452.
- [19] J. J. Martinez and P. T. Esperana. A Chebyshev collocation spectral method for numerical simulation of incompressible flow problems. Journal of the Brazilian Society of Mechanical Sciences and Engineering, 29(3), 2007, 317-328.
- [20] T. Saitoh and K. Hirose. High-accuracy bench mark solutions to natural convection in a square cavity. Computational Mechanics, Vol. 4, 1989, 417-427
- [21] J. D. Anderson Jr. Computational Fluid Dynamics: The Basics with Applications. McGraw-Hill, NewYork, 1995.