Titel

Master-Thesis von Fabian Nuraddin Alexander Gabel
Tag der Einreichung:

1. Gutachten: Prof. Dr. rer.nat. Michael Schäfer
2. Gutachten: Dipl.-Ing Ulrich Falk

TECHNISCHE UNIVERSITÄT DARMSTADT

Studienbereich CE
FNB

Titel

Vorgelegte Master-Thesis von Fabian Nuraddin Alexander Gabel

1. Gutachten: Prof. Dr. rer.nat. Michael Schäfer
2. Gutachten: Dipl.-Ing Ulrich Falk

Tag der Einreichung:

Erklärung zur Master-Thesis

Hiermit versichere ich, die vorliegende Master-Thesis ohne Hilfe Dritter nur mit den angegebenen Quellen und Hilfsmitteln angefertigt zu haben. Alle Stellen, die aus Quellen entnommen wurden, sind als solche kenntlich gemacht. Diese Arbeit hat in gleicher oder ähnlicher Form noch keiner Prüfungsbehörde vorgelegen.

Darmstadt, den November 23, 2014

(F. Gabel)

Contents

1 Introduction

This thesis is about.

2 Fundamentals of Continuum Physics for Thermo-Hydrodynamical Problems

2.1 Navier-Stokes Equations for Incompressible Flows

2.1.1 Cauchy-Equations

2.1.2 Newtonian Fluids

2.1.3 Final Form of the Navier-Stokes Equations - conservative and nonconservative Form

2.2 Energy Equation

2.2.1 Generic Scalar Transport Equation

2.2.2 Bouyancy Driven Flows - Densities as Functions of the Temperature

3 Finite Volume Methods for Incompressible Flows - Their Theoretical Basics and their Realisation in Code

3.1 Fundamentals of Discretisation

3.1.1 Numerical Grid

3.1.2 Approximation of Integrals

3.2 Discretisation of the Momentum Balance

3.2.1 Semi Discretized Linearized Form of the Navier-Stokes Equations

3.2.2 Treatment of Nonorthogonalities

3.2.3 Calculation of Mass Flux - Rhie-Chow Interpolation

3.2.4 Discretization of the convective term

3.2.5 Discretization of the diffusive term

3.2.6 Discretisation of the source term

3.2.7 Assembly of Linear Systems - Final Form of Equations

3.3 Discretisation of the Generic Transport Equation

3.4 Segregated Methods - SIMPLE Algorithm

3.4.1 Pressure Correction Equation

3.4.2 Characteristical Properties of Projection Methods

Underrelaxation, slow convergence, inner iterations outer iterations, relative tolerances

3.5 Boundary Conditions on Domain and Block Boundaries

3.5.1 Dirichlet Boundary Condition

3.5.2 von Neumann Boundary Condition

3.5.3 Symmetry Boundary Condition

3.5.4 Wall Boundary Condition

3.5.5 Block Boundary Condition

3.6 Coupled Solution of the Navier-Stokes Equations

3.6.1 Discretization fo the Navier-Stokes Equations

3.6.2 Differences to the segregated approach

Implicit treatment of Pressure Gradient, Implicit treatment of Temperature

3.6.3 Assembly of Linear System

3.6.4 Boundary Conditions

3.7 Characteristical Properties of the coupled solution approach

Bad condition, singularity, faster convergence

3.8 Numerical Solution of Linear Systems

3.8.1 Stone's SIP Solver

Basic Idea

3.8.2 Krylov Subspace Methods

Basic Idea, some representative algorithms, importance of preconditioning

4 CAFFA Framework

4.1 PETSc Framework

Keep in mind not to copy the manual but

4.1.1 Philosophy of PETSc

Bell Prize, MPI Programming

4.1.2 Basic Data Types

Vec,Mat (Different Matrix Types and their effect on complex methods)

4.1.3 KSP and PC Objects and their usage

Singularities

4.1.4 Profiling

Petsc Log

4.1.5 Common Errors

Optimization, Interfaces, Compiler Erros not helpful, Preallocation vs. Mallocs

4.2 Grid Generation and Conversion

Generation of block structured grids, neighbouring relations are represented by a special type of boundary conditions

4.3 Preprocessing

Matching algorithm - the idea behind clipper. Opencascade. Efficient calculation of values for discretization.

4.4 CAFFA3D

4.4.1 MPI Programming Model

4.4.2 Indexing of variables and treatment of boundary values

Describe MatZeroValues and how it is used to simplify the code. Problems with boundary entries

4.4.3 Field interlacing

Realization through special arrangement of variables and the use of index sets and/or preprocessor directives

4.4.4 Domain Decomposition, Ghosting and Parallel Matrix Assembly

Ghost values are stored in local representations of the global vector (state the mapping for those entries). Matrix coefficients are calculated on one processor and sent to the neighbour. Preallocation as crucial aspect for program performance.

4.5 Postprocessing

Visualization of Results with Paraview and Tecplot

5 Verification of CAFFA

5.1 Theoretical Discretisation Error

5.2 Method of Manufactured Solutions

5.3 Exact and Manufactured Solutions for the Navier-Stokes Equations and the Energy Equation

Not always there is an exact solution. Divergence free approach. Presentation of the used manufactured solution.

- `http://scicomp.stackexchange.com/questions/6943/manufactured-solutions-for-incompressible-navier-stokes`
- `http://link.springer.com/article/10.1007/BF00948290`
- `http://physics.stackexchange.com/questions/60476/exact-solutions-to-the-navier-stokes-equations`
- `http://www.annualreviews.org/doi/pdf/10.1146/annurev.fl.23.010191.001111`

5.4 Measurement of Error and Calculation of Order

6 Comparison of Solver Concepts

6.1 Impact on Convergence Behaviour on Blockstructured Grids

Show how the implicit treatment of block boundaries maintains high convergence rates

6.2 Parallel Performance

6.2.1 Cluster Hardware and Used Software

- Mem Section and processes in between islands (calculating across islands)
- Versioning information (PETSc,INTEL COMPILERS,CLIPPER,MPI IMPLEMENTATION)
- Software not designed to perform well on desktop PCs.

6.2.2 Measures of Performance

- Maße definieren
- Nochmal Hager,Wellein studieren
- Guidelines for measuring performance (bias through system processes or user interaction), only measure calculation time do not consider I/O in the beginning and the end

6.2.3 Preiliminary upper bounds on performance - The STREAM Benchmark

Pinning of processes, preiliminary constraints by hardware and operating systems, identification of bottlenecks, history and results of STREAM

6.3 Discussion of Results for Parallel Efficiency

6.4 Speedup Measurement for analytic Testcases

6.5 Convergence Behaviour

6.6 Application in Realistic Testcases

6.6.1 Flow around a cylinder 3d - stationary

6.6.2 Flow around a cylinder 3d - instationary

- `http://www.featflow.de/en/benchmarks/cfdbenchmarking/flow/dfg_flow3d/dfg_flow3d_configuration.html`

6.6.3 Heat-Driven Cavity Flow

- `http://www.featflow.de/en/benchmarks/cfdbenchmarking/mit_benchmark.html`

7 Conclusion