Implementation and Performance Analyses of a Highly Efficient Algorithm for Pressure-Velocity Coupling

Implementierung und Untersuchung einer hoch effizienten Methode zur Druck-Geschwindigkeits-Kopplung

Master-Thesis von Fabian Nuraddin Alexander Gabel

Tag der Einreichung:

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2. Gutachten: Dipl.-Ing Ulrich Falk

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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 28, 2014

(F. Gabel)

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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

2.3 Bouyancy Driven Flows - the Boussinesq Approximatio

Talk about natural and forced convection. Differences for the solver algorithm. (s.a.) Peric P447 Talk abourt flows with variation in fluid properties -> mms has to map this behaviour (bouyancy force driven, i.e. naturally convected fluid) Also talk about nondimensional values like prandtl number, rayleigh and reynolds

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

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3.2.1 Semi Discretized Linearized Form of the Navier-Stokes Equations

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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 - the 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 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 of the Navier-Stokes Equations

3.6.2 Differences to the Segregated Approach - Implicit Coupling of Velocities, Pressure and Temperature

Implicit treatment of Pressure Gradient, Implicit Treatment of Temperature possible, boussinesq approximation brings maximal coupling. Temperature dependent densities also possible

3.6.3 Assembly of Linear System

3.6.4 Boundary Conditions

3.7 Characteristical Properties of the Fully Coupled Solution Approach

Bad condition, singularity, faster convergence, coupling in bouyancy flows (s.a. Peric page 448, Galpin Raithby)

3.8 Numerical Solution of Linear Systems

3.8.1 Stone's SIP Solver

Basic Idea as in Schäfer or Peric

3.8.2 Krylov Subspace Methods

General concept of cyclic vector spaces of $\mathbb{R}^n$, name some representative ksp algorithms, importance of preconditioning, not as detailed as in bachelor thesis

4 CAFFA Framework

4.1 PETSc Framework

Keep in mind not to copy the manual but

4.1.1 About 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 and the used projection technique; alt.: Opencascade. Efficient calculation of values for discretization.

4.4 CAFFA3D

4.4.1 MPI Programming Model

Basic idea of distributed memory programming model, emphasize the differences to shared memory model

4.4.2 Indexing of Variables and Treatment of Boundary Values

Describe MatZeroValues and how it is used to simplify the code. Compliance of PETSc zero based indexing and CAFFA indexing which considers boundary values. Problems with boundary entries

4.4.3 Field Interlacing

Realization through special arrangement of variables and the use of index sets (subvector objects) and/or preprocessor directives. Advantages (there was a paper I cited in my thesis)

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. Present a simple method for balancing the matrix related load by letting PETSc take care of matrix distribution.

4.5 Postprocessing

Visualization of Results with Paraview and Tecplot

5 Verification of CAFFA

Refer to next section for Validation of CAFFA

5.1 Theoretical Discretisation Error

present the Taylor-Series Expansion

5.2 Method of Manufactured Solutions

basically sum up the important points of salari's technical report, symmetry of solution/domain/grid is bad point out that mms is not able to detect errors in the physical model

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. What if solution is not divergence free? Derivation of equations and modifications to continuity equation. analyze the problem of too complicated manufactured solutions. also use temperature dependent density function

- `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

Different error measures (L2-Norm,completeness of function space, consistency etc.)

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. Plot Residual over number of iterations.

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,BLAS/LAPACK)
- 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
- Cite Schäfer and Peric with their different indicators for parallel efficiency, load balancing and numerical efficiency

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. Bandwith as Bottleneck. Petsc Implementation of STREAM

6.3 Discussion of Results for Parallel Efficiency

6.4 Speedup Measurement for Analytic Testcases

6.5 Application to Testcases with Varying Degree of Non-Linearity

As Peric says I want to prove that the higher the nonlinearity of NS, the better relative convergence rates can be achieved with a coupled solver. Fi

6.5.1 Transport of a Passive Scalar - Forced Convection

6.5.2 Bouyancy Driven Flow - Natural Convection

6.5.3 Flow with Temperature Dependent Density - A Highly Nonlinear Testcase

6.6 Comparison of Solver Concepts in Realistic Scenarios

Also consider simple load balancing by distributing matrix rows equally

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 and Outlook

Turbulence, Multiphase, GPU-Accelerators, Load-Balancing, dynamic mesh refinement, Counjugate Heat Transfer with other requirements for the numerical grid, grid movement