NTNU

Project TMA4500

Least Squares Method

Author:
Magnus Aarskaug Rud

Supervisor:
Anne Kværnø

Research Group Name
IMF

October 2015

NTNU

Abstract

Faculty Name
IMF

Project TMA4500

Least Squares Method

by Magnus Aarskaug Rud

In this project some basic properties of the least squares method is analysed. Both finite element and spectral methods are discussed, and the implementation is mainly performed using spectral basis functions. The problems analysed in this project are diffusion convection reaction PDEs, both linear and non-linear. The results are compared to standard Galerkin method where both error and condition number is considered. The least squares method is also applied to Galerkin methods to gain stability with great results.

Contents

Abstract **i**

Contents **ii**

Notation **iii**

1 Numerical theory **1**
1.1 Galerkin formulation 1
1.2 Finite element method 2
1.3 Spectral methods 3
1.4 Spectral element method 4

2 Fluid dynamics and problem specific mathematics **5**
2.1 Navier-Stokes equation 5
2.2 Resolving the turbulent term 6
2.3 Solution methods of incombressible N-S 7
2.4 nek5000 7

3 Application of nek5000 and the creation of grid **8**
3.1 Nek5000 8
3.2 Gas dispersion in a simplified urban area 9
3.3 Creation of the mesh-convertion script 9

Notation

CONVENTION we let subscript h denote the discretized variables

Chapter 1

Numerical theory

1.1 Galerkin formulation

Throughout this thesis all numerical methods will be based on the Galerkin formulation. Let us consider a general bounary value problem (BVP)

$$\begin{aligned} \mathcal{L}u =& f \quad \text{in } \Omega \\ \mathcal{B}u =& g \quad \text{on } \partial\Omega. \end{aligned} \tag{1.1}$$

The domain Ω is a closed subspace of $\mathbb{R}^d$, $\mathcal{L} : X(\Omega) \to Y(\Omega)$ and $\mathcal{B} : X(\partial\Omega) \to B(\partial\Omega)$ are two linear operators, $f \in Y(\Omega)$ and $g \in B(\partial\Omega)$ are known functions and $u \in X(\Omega)$ is the wanted solution. The space $X(\Omega)$ is called the search space. A weak formulation can now be obtained by multiplying the first equation in 1.1 by a test function $v \in X^t(\Omega)$ and integrating over the domain Ω. By choosing $X^t(\Omega) = X(\Omega)$ the Galerkin formulation is obtained. For more examples and information on this subject the first chapters in [1] are recommended.

By the Lax-Milgram theorem it is known that a BVP is well-posed if the Operator $\mathcal{L}$ is both bounded and coersive.

- a common BVP, weak formulation
- search and solution space, test and basis functions
- error estimation

1.2 Finite element method

Finite element method is one of the most widely used numerical methods applied on problems within construction, flow simulation and many other areas. It offers a precise mathematical foundation and due to the connectivity properties of the elements it guaranties a sparse system. The decomposition of the geometrical domain into a finite amount of elements chosen according to the problem wanted to solve, makes it possible to create general algorithms applicable to all kinds of geometries. For the full mathematical foundation of FEM it will be referred to [1], but some of the key propertie will be stated here in order to provide a thourough understanding of the spectral element method.

FEM provides an alorithm for solving any BVP 1.1 and the mathematical formulation is obtained by first finding the Galerkin formulation and then choosing a discrete subset $X^h(\Omega) \subset X(\Omega)$ as your search space. Another key aspect of FEM is the treatment of the domain Ω, on which a triangulization $\{\mathcal{T}_h\}$ is defined such that the original domain is divided into elements. The discrete subset X^h is defined by a particular basis. FEM is called a projection method since the solution $u_h \in X^h$ is a projection of the actual solution u of the BVP onto the discrete space X^h. ——— DEFINE THIS NICER — ————- The basis functions of FEM are known as hat functions and allthough there are many possible choices they are defined such that all elements consists of the same "local" basis functions, and the global basis functions are non-zero in only a small part of Ω. The first feature enables us to develop a local routine performed on each element and later assemble all the local information in a global system of equations.

The numerical error of FEM is reduced to the order of the approximation error of a function from X to X^h. error estimation

Before this section ends it is important to understand the two ways to improve the error and the effects these two ways have on the algorithm. Assume the solution of the BVP to be infinitely smooth and let h denote the geneal size of the elements and p the order of the polynomial basis that defines X^h. performing a h-refinement will lead to a convergence of h^p, sparsity of the system is conserved and the total algorithm does not change in any other way than increasing the number of elements. Keeping h constant and increasing p will provide spectral convergence, but the sparsity will be reduced and all integrals solved will require quadrature rules of higher order.

- projection onto a h-subspace
- the basis functions
- convergence rate
- How the sparsity decays with increasing polynomial order
- assembly algorithm
- problem with a non-symmetrical problem

1.3 Spectral methods

Spectral methods share a some of the mathematical ideas as FEM, but are not as widely used in real life problems. SM are however very interesting from a theoretical point of view due to its spectral convergence rate which allows you to obtain solutions of extremely high accuracy. The most important draw-back of SM are the difficulties with applications to complex geometries. Allthough the system of equations surging from a BVP can be constructed in an elegant way it is rarely sparse and often result in expensive calculations.

- quadrature rule
- the choice of nodes and basis functions
- the role of the jacobian
- cross product formulations

[2]

1.4 Spectral element method

In the early 1980's the the idea to combine FEM and SM came along in order to obtain the robustness and resulting sparse system of FEM and the spectral convergence rate provided by SM. The result was the Spectral element method. Read articles... Several formulations was investigated and the development of super computers has played an important role in deciding the method applied today. The basic idea is to divide the domain of the BVP wanted to solve into elements as in FEM and then use spectral basis functions of higher degree with support only within one element.

- READ LITERATURE ON THIS !!

Chapter 2

Fluid dynamics and problem specific mathematics

2.1 Navier-Stokes equation

The physics regarding fluids in motion are described mathematically by the Navier-Stokes equation. The equations can be derived in many ways, and it is referred to [**?**] for a complete explication. The general idea is to conserve momentum and mass in a control domain and by applying Reynolds transport theorem and the result is the following two equations reffered to as the N-S equations.

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}(\nabla \cdot \mathbf{u}) = -\nabla p + \nu \nabla \cdot \tau \tag{2.1}$$

$$\nabla \cdot (\rho \mathbf{u}) = 0 \tag{2.2}$$

These equations have been studied for centuries and different physical situations lead to different simplifications and sets of equations. Examples are the Euler equations, Stokes problem, darcy flow and the incompressible navier-stokes equations. Without doing the derivation of the equations a short discussion of each term in equation N-S will be given here in order to understand there physical origin and their mathematical attributes.

The term $\partial\mathbf{u}/\partial t$ is the time-derivative of the flow, for a steady state flow this term will be equal zero. The discretization of this term is often based on some implicit scheme.

The convective term $\mathbf{u}(\nabla \cdot \mathbf{u})$ describes the transport due to the flow itself on each of its components. This term is non-linear and does therefore require the equations to be solved by some iteration procedure such as Newton iterations.

The diffusive term $\nu\Delta\mathbf{u}$ describes the natural diffusion of the fluid. The effect of diffusion is determined by the viscosity of the fluid. Mathematically this term makes the equations numerically stable and it is therefore generally easier to solve the N-S equations for high-viscosity fluids.

The pressure gradient ∇p is the only term involving the pressure, ... DISCUST THE MEANING OF PRESSURE... in modern solution techniques it is common to solve eq. 2.2 in a decoupled manner.

The reynolds stress tensor $\tau = \cdots$ is the turbulent term of the N-S equation. In laminar flow this term can be neglected.

The second equation in 2.2 imposes a divergence free constraint on the solution $\mathbf{u}$ if the fluid is assumed to be incombressible. The density ρ will be a constant and the simplification follows trivially.

The coefficient ν is the inverse Reynolds number $1/Re$,

- The time-derivative
- The convective term
- The diffusive term
- The pressure gradient
- The reynolds stress tensor
- The reynolds number
- The mass equation

2.2 Resolving the turbulent term

Depending on the wanted accuracy of your solution and the number of computational units at hand the turbulent term can be solved in different ways. A brief overview of the different approaches to the turbulent term are discussed in the following subsections

- Laminar flow
- RANS
- LES
- K-epsilon and K-omega
- DNS

2.3 Solution methods of incombressible N-S

A non-linear set of equations requires a non-trivial solution method, and when the domain of the problem can be anyting from a simple channel to a moving turbine there are many considerations that needs to be made. Allthough the equations have been known for over 200 years no one has been able to prove or disprove the well-posedness of the problem. FINAL ELEMENT FORMULATION WELL-POSED?? Some of the most common algorithms will be discussed in the following subsections

- coupled versus decoupled
- The Uzawa algorithm
- Pressure correction method
- fractional step method

2.4 nek5000

Nek5000 is a turbulent flow solver developed mainly by Paul Fischer and has through the past 20 years had several contributours. It is a open-source code applicable to many different flow situations.

- Application areas
- Description of the numerical algorithm
- usage of the program

Chapter 3

Application of nek5000 and the creation of grid

3.1 Nek5000

There are many numerical solvers for turbulent flows available on the market. From large commercial softwares such as fluent which runs as a black-box solver, to CDP which is a bit more specialized solver with the posibility to modify the code to apply it to the wanted usage and to full open-source codes such as nek5000 and openFOAM. The solvers can vary both in the fundamental numerical method (FV,FD,FEM,SEM) the implemented algorithm (Fractional Step, Poisson pressure, Uzawa) and the type of simulation (RANS,LES,DNS). The software is chosen depending on the users requirement, but the work flow does follow a certain structure in all cases.

- Practical problem –¿ Mathematical formulation –¿ Generation of mesh –¿ Simulation –¿ post-processing

An example is waterflow in a channel, which would be the practical problem. The mathematical formulation would be the incompressible N-S eq, with LES dynamical SGS. The mesh could consist of tetrahedros or hexahedrons. The simulation is the performed on some cluster before the wanted data in some sub-domain is visualized and presented.

Nek provides a basic tool for generation of mesh. For more complex geometries this tool cannot compare with more visualized-based softwares such as ICEM from ANSYS which exports mesh to several numerical solvers such as Fluent and nastran. It is therefore very useful to have an automatic way of converting a mesh created in ICEM to the format required by nek5000. In order for nek to run optimally the elements should be as homogenous and as similar to the reference element as possible. It is therefore of great interest to be able to propagate curved geometries into the neighbour-elements in order to have a smooth as possible transition from a boundary with high curvature.

3.2 Gas dispersion in a simplified urban area

The problem investigated in this work is gas dispersion of neutral gas in a velocity field through four cubic blocks. Similar simulations have been done in CDP and Fluent which are compared to data from a wind-tunnel experiment performed by ALAN.

- Description of problem and domain
- mesh and fluent/CDP mesh

3.3 Creation of the mesh-convertion script

- initial script
- changes and modifications
- performance testing
- pitfalls

Bibliography

[1] Alfio Quarteroni. *Numerical Models for Differential Problems, 2. edition*. Springer, 2014.

[2] C. Canuto and A. Quarteroni. Approximation results for orthogonal polynomials in sobolev spaces. *Mathematics of Computation*, 38(157):67–67, Jan 1982. ISSN 0025-5718. doi: 10.1090/s0025-5718-1982-0637287-3. URL http://dx.doi.org/10.1090/S0025-5718-1982-0637287-3.