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Termination criteria for GMRES-like methods to solve the discretized incompressible Navier-Stokes equations

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Abstract

In this paper we discuss some strategies to solve the discretized incompressible Navier-Stokes equations in general coordinates. For the implicit time integration a termination criterion is given, and some practical and theoretical properties of this criterion are shown. The linear systems: momentum-, pressure- and transport equations are solved each timestep by an iterative solution method (GMRES). We specify and discuss several starting- and stopping strategies. Some numerical experiments are used to illustrate the theory. These experiments show that a clever solution strategy can save much CPU-time.

1 Introduction

In this paper we summarize the state of the art of our incompressible Navier-Stokes solver. We focus attention on the solution of stationary problems. In all sections we end with suggestions for further research.

We consider the flow of an incompressible fluid in a two dimensional domain. In[4] and [13] the Navier-Stokes equations, which are used to describe this flow, are formulated in general coordinates. We present these equations in Cartesian coordinates:

$$\frac{\partial u_i}{\partial t} - \left(\frac{\partial \tau_{i1}}{\partial x_1} + \frac{\partial \tau_{i2}}{\partial x_2}\right) + \frac{\partial u_i u_1}{\partial x_1} + \frac{\partial u_i u_2}{\partial x_2} + \frac{\partial p}{\partial x_i} = 0, \;\; i \in \{1,2\},$$

where

$$\tau_{ii} = Re^{-1}\left(\frac{4}{3}\frac{\partial u_i}{\partial x_i} - \frac{2}{3}\frac{\partial u_j}{\partial x_j}\right),\; \tau_{ij} = Re^{-1}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right),\; i,j \in \{1,2\},\; i \neq j,$$

together with the incompressibility condition

$$\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} = 0,$$

and appropriate initial and boundary conditions. In these equations u_i is the component of the velocity of the fluid in x_i-direction, p is the pressure and Re the dimensionless Reynolds number.

With respect to the time-discretization, we restrict ourselves in this paper to the Euler backward scheme in combination with a pressure correction method [15], and a Newton linearization. The timestep is denoted by Δt. For a given function v and $n \in I\!N$, v^n is an approximation of $v(n\Delta t)$.

For the discretization in space the physical domain is mapped onto a rectangle (computational domain). Combining this coordinate transformation with finite volumes on a staggered grid in the computational domain, we obtain two systems of equations:

the momentum equations:
$$M^{n+1}u^{n+1} = f^{n+1},\ u^{n+1} = \begin{pmatrix} u_1^{n+1} \\ u_2^{n+1} \end{pmatrix}, \tag{1}$$

and the pressure equation:
$$P\Delta p^{n+1} = g^{n+1},\ \text{where } \Delta p^{n+1} = p^{n+1} - p^n. \tag{2}$$

For more details on the discretization we refer to [4] and [13]. More details on iterative solution methods to solve these systems of equations are given in: [17] using Krylov subspace methods, and [5], [8] using multigrid methods. A comparable discretization of the incompressible Navier-Stokes equations in general coordinates is given in [10]. They use a multigrid method to solve their linear systems of equations [9].

Other iterative methods to solve the incompressible Navier-Stokes equations are:

- the SIMPLE method (Semi-Implicit Method for Pressure-Linked Equations) [7], [6],
- the distributive Gauss-Seidel smoothing method [1], [2],
- the symmetric coupled Gauss-Seidel method [16],
- the distributive ILU smoothing method [20].

For more details on these methods used in combination with the mutigrid method we also refer to [19].

In Section 2 we specify a test problem, which will be used throughout this paper. We consider some quantities to measure the convergence of the time dependent solution to the stationary solution. These quantities are used in a termination criterion. The section is illustrated with some numerical experiments for different Reynolds numbers (Re) and timesteps (Δt).

In Section 3 the momentum equations are solved with an iterative solution method.We discuss some termination criteria. From numerical experiments we obtain relations between the termination criteria of the sections 1 and 2. Furthermore, these experiments show the behaviour of GMRES, an iterative solution method proposed in [11], for different choices of Re and Δt. Thereafter we approximate the eigenvalues of the discretized momentum equations. We show that these approximations can be used to study the stability of the time integration, and the convergence behaviour of the iterative solution method.

The pressure equations are solved in Section 4 with a new variant of GMRES: GMRESR. One of the given termination criteria relates the accuracy of the approximate pressure solution to the divergence of the resulting velocity field. Initially we start GMRESR with a start vector equal to zero. It appears that other start vectors give a faster convergence of GMRESR.
Our experiments show that a clever combination of starting, postconditioning and termination strategies may result in a considerable saving in CPU time.

Finally, in Section 5 we consider the case of a transport equation, coupled with the Navier-Stokes equations. The structure of the discretized transport equation is the same as the structure of the pressure equation, whereas the convergence behaviour of GMRES is the same as for the momentum equations. Starting vectors and termination criteria are given.

2 The time integration

In this section we describe the geometry and initial and boundary conditions for the test problem that is used in the remainder of this paper. We specify some quantities to observe the convergence of the time dependent solution to the stationary solution. Furthermore, these quantities are used to define a termination criterion, which implies that the distance between the calculated solution and the stationary solution is less than a prescribed quantity. Finally, we give some theoretical and practical properties of the termination criterion.

The test problem describes the flow through a curved channel. The physical domain is displayed in Figure 1. As initial condition we take the velocities equal to zero. The following boundary conditions are used: a parabolic velocity profile, with the maximum velocity equal to one at the inflow boundary (Boundary 1), a no slip condition on Boundary 2 and 4, and the normal stress and tangential velocity given on the outflow boundary (Boundary 3). The total number of finite volumes in our example is $16 \times 64 = 1024$.

In this paper we are interested in the stationary solution. To compute this solution we use the time-dependent equations, and try to obtain the stationary solution in a cheap way. This means that we stop the time integration as soon as possible, and choose a large time step Δt.

In the following we state some theoretical results, which are used to obtain a practical termination criterion. If this criterion holds we expect that the solution no longer depends on the time variable, and is a good approximation of the stationary solution.

We define ρ_u^i as follows: $\rho_u^i = \frac{\|u^i - u^{i-1}\|_2}{\|u^{i-1} - u^{i-2}\|_2}$. To obtain a termination criterion we assume that ρ_u exists such that:

$$\rho_u^i \leq \rho_u < 1 \text{ for all } i. \tag{3}$$

Under certain conditions it is possible to prove that ρ_u exists, however, in practice these conditions can be too severe. In such a case it is always possible to inspect ρ_u^i after n timesteps, and look, for a $\rho_u > 0$ such that $|\rho_u^i - \rho_u| < \delta \ll 1 - \rho_u$, for $i \in [n-m, n]$. For large m, it is reasonable to assume that inequality (3) holds for all $i \geq n - m$. In Figure 2 we show ρ_u^i and $\rho_u = 0.81$ for $Re = 10, \Delta t = 0.0625$ and $n = 40$. Note that $\|\rho_u^i - \rho_u\|_2 \ll 1 - \rho_u$ for $i \in [15, 39]$.

The stationary solution is denoted by $u = \lim_{i \to \infty} u^i$. Using (3) we obtain the following inequalities for $k \geq i + 1 > n - m$:

$$\|u^k - u^i\|_2 \leq \sum_{j=i}^{k-1} \|u^{j+1} - u^j\|_2 \leq \sum_{j=1}^{k-i} \rho_u^j \|u^i - u^{i-1}\|_2$$

$$= \rho_u \frac{1 - \rho_u^{k-i-1}}{1 - \rho_u} \|u^i - u^{i-1}\|_2,$$

which implies $\|u - u^i\|_2 \leq \frac{\rho_u}{1-\rho_u} \|u^i - u^{i-1}\|_2$. This leads to the following termination strategy: compute ρ_u^i, estimate ρ_u such that (3) holds, and stop if

$$\frac{\rho_u}{1 - \rho_u} \frac{\|u^i - u^{i-1}\|_2}{\|u^i\|_2} \leq \varepsilon. \tag{4}$$

Using this termination criterion it follows that

$$\frac{\|u - u^i\|_2}{\|u\|_2} \cong \frac{\|u - u^i\|_2}{\|u^i\|_2} \leq \frac{\rho_u}{1 - \rho_u} \frac{\|u^i - u^{i-1}\|_2}{\|u^i\|_2} \leq \varepsilon,$$

so the relative error in u^i is less than ε. For the pressure we define $\rho_p^i = \frac{\|p^i - p^{i-1}\|_2}{\|p^{i-1} - p^{i-2}\|_2}$ and use an equivalent termination strategy (see also [12]; p.13).

Some topics for further research are:

- how to obtain a good choice of Δt,
- is it a good idea to take Δt as a function of the time variable?
- the behaviour of ρ_u and ρ_p in relation with $\Delta t, Re$, etc,
- the convergence behaviour to the stationary solution.

In the following paragraphs we describe some experiments to illustrate the above mentioned topics. Figure 3 and 4 show the quantities:

$^{10}\log\left(\frac{\rho_u}{1-\rho_u} \frac{\|u^i - u^{i-1}\|_2}{\|u^i\|_2}\right)$ respectively $^{10}\log\left(\frac{\rho_p}{1-\rho_p} \frac{\|p^i - p^{i-1}\|_2}{\|p^i\|_2}\right)$,

for our testproblem with $\Delta t = 0.125, T = 10$ and various choices of Re. For $Re \leq 10$ we observe a reasonably smooth convergence behaviour. Note that $Re = 10$ converges much faster than $Re = 1$. Considering the convergence of u^{i+1} for $Re = 50$ or 100 we see that initially convergence is much slower for $Re = 50$ or 100 than $Re \leq 10$, but after some time convergence is faster. Comparing $Re = 50$ and 100 we note that $Re = 100$ converges slower than $Re = 50$. A possibility to obtain a smoother behaviour for $Re = 50$ and 100 is to start with a smaller timestep Δt and after some steps to enlarge it.

Figures 5 and 6 show the same quantities for $Re = 10, \Delta t = 0.25, 0.125$ and 0.0625. Note that $\Delta t = 0.25$ shows a bad convergence behaviour especially in the convergence of the pressure. With respect to the choice $\Delta t_1 = 0.125$ and $\Delta t_2 = 0.0625$ we note that one time step with Δt_2 is cheaper than with Δt_1, because the starting solutions are better and the momentum equations have a better convergence behaviour. It appears from the following examples that a too large choice of Δt leads to much CPU-time to obtain a stationary solution. For instance, if we choose $\varepsilon = 10^{-3.8}$ for the momentum equations than it follows from Figures 3 and 5 that we need 45 steps for $\Delta t_2 = 0.0625$ and 64 steps for $\Delta t_1 = 0.125$. For the pressure equation we choose $\varepsilon = 10^{-2.5}$ and need 24 steps with Δt_2 and 36 steps with Δt_1. For both choices of ε using the small time step Δt_2 costs much less work than the choice Δt_1.

Conclusions

In this section we specify termination criteria to stop the time integration. The termination criteria are shown to be correct if the assumption $\rho_u^i \leq \rho_u < 1$ holds for all i. Although we are not able to prove that in our examples this assumption is satisfied, we note that in many cases ρ_u^i converges to a quantity $\rho_u < 1$ and thus the assumption is correct for i large enough. In some experiments ρ_u^i does not converge or $\rho \geq 1$. This gives useful information too, because it indicates that the computed solution u^i does not converge to a stationary solution u. In many cases this defect is cured if we take a smaller timestep Δt. In Section 3.5 we shall analyse a problem where also for a smaller timestep Δt there is no $\rho_u < 1$ such that $\rho_u^i \to \rho_u$. It appears that in this experiment the Euler backward integration scheme is unstable.

3 The momentum equations

In this section we solve the momentum equations with an iterative solution method: GMRES. It is necessary to stop the iterative method if a certain accuracy is obtained. In the first part of this section we discuss several termination criteria. In the second part we give the Ritzvalues, which are approximations of the eigenvalues of the momentum equations, for different choices of the Reynolds number and the timestep.

3.1 Termination criteria

Consider the linear system $Ax = b$. If x_j is an approximation obtained with an iterative solution method, the following termination criteria are usually applied. Define $r_j = b - Ax_j$ the residual of the iteration process.

Criterion 1: $\|r_j\|_2 < \varepsilon$.
The main disadvantage of this criterion is that it is not scaling invariant. So a correct choice of ε depends on properties of the matrix A.

Criterion 2: $\|r_j\|_2 / \|r_0\|_2 < \varepsilon$.

This criterion is scaling invariant. However, the number of iterations is independent of the initial estimate x_0. This can be a drawback, because we expect that after some time, the solution of the preceding timestep is a good starting solution.

Criterion 3: $\|r_j\|_2/\|b\|_2 < \varepsilon$.
This is a good criterion, because it is scaling invariant, and if the iteration process is started with an accurate solution vector the number of iterations is less than using an inaccurate start vector.

Criterion 4: $K_2(A)\|r_j\|_2/\|b\|_2 < \varepsilon$.
From the inequality $\frac{\|x-x_j\|_2}{\|x\|_2} \leq K_2(A)\frac{\|r_j\|_2}{\|b\|_2}$, it follows that if the iteration process is stoped using Criterion 4 then $\frac{\|x-x_j\|_2}{\|x\|_2} \leq \varepsilon$.
So this is the best termination criterion, since the iteration process stops if the norm of the error with respect to the norm of the solution is less than a prescribed accuracy. However, in general, $K_2(A)$ is not known.

The foregoing discussion motivates us to use the GMRES method [11] combined with the criterion

$$\frac{K_2(M^{n+1})\|r_j\|_2}{\|f^{n+1}\|_2} < \varepsilon_u$$

to solve the momentum equations $M^{n+1}u^{n+1} = f^{n+1}$. To obtain an estimate for $K_2(M^{n+1})$ we calculate the singular values of $R_j \in \mathbb{R}^{(j+1)\times j}$. The matrix R_j is automatically computed in the GMRES method and hence there is no overhead (see [11], p. 861). An underestimate of $K_2(M^{n+1})$ is given by the ratio $\sigma_1^{(j)}/\sigma_j^{(j)}$ where $\sigma_1^{(j)}$ is the largest and $\sigma_j^{(j)}$ the smallest singular value of R_j. It appears that in many applications $\sigma_1^{(10)}/\sigma_{10}^{(10)}$ is a good approximation of $K_2(M^{n+1})$ ([17], p. 11). So we use the following termination strategy, which is a combination of Criterion 3 and 4: the GMRES method is stopped if $j < 10$ and $\frac{\|r_j\|_2}{\|f^{n+1}\|_2} < \varepsilon_u$, or $\frac{\sigma_1^{(10)}}{\sigma_{10}^{(10)}}\frac{\|r_j\|_2}{\|f^{n+1}\|_2} < \varepsilon_u$.

3.2 Numerical experiments

Although a good choice of ε_u is unknown and subject of further research, we use $\varepsilon_u = 10^{-5}$, which appears to be a reasonable choice in our experiments. In the following paragraphs we discuss the results of our experiments.

Influence of the starting solution
In Figure 7 and 8 the number of GMRES iterations to approximate the solution of the momentum equations are shown. Note that after some timesteps the number of iterations decreases considerably. An explanation of this behaviour is that after some time the initial approximation becomes better and better, so it costs fewer iterations to satisfy our termination criterion. We have also tried to make a better initial estimate by using the following extrapolation:

$$u^{n+1} \simeq u^n + \Delta t\frac{du^n}{dt},$$

and approximating $\frac{du^n}{dt}$ by $\frac{u^n - u^{n-1}}{\Delta t}$. In this way we get the following initial estimate $u_0^{n+1} = u^n + \Delta t \frac{u^n - u^{n-1}}{\Delta t} = 2u^n - u^{n-1}$. The decrease in the number of iterations was small (a gain of one or two iterations). For that reason we have decided to limit ourselves to the case in which we start with $u_0^{n+1} = u^n$.

Influence of Δt

From Figure 3.2 it appears that a reduction of the timestep Δt gives a faster convergence of the GMRES method. This is expected because if Δt goes to zero, the eigenvalues of $\frac{\Delta t}{\rho} M^{n+1}$ cluster around 1, and it is well known that GMRES converges very fast for matrices where the eigenvalues are clusteed. Moreover, if Δt decreases the initial estimate $u_0^{n+1} = u^n$ becomes better.

The choice of ε_u

For $Re = 50, \Delta t = 0.125$ and $Re = 10, \Delta t = 0.0625$ we see after some timesteps that the number of GMRES iterations is equal to zero. This means that the solution is constant in the time variable, and no longer converges to the stationary solution. However the termination criterion for the time integration is not satisfied. To get around this it seems a good idea to enforce a minimum number of GMRES iterations, say 3.

Irregularities in the converence of the time integration

We observe in Figure 3 some irregularities in the convergence of the time integration. For instance for $Re = 10$, there are disturbances at $t = 3.6$ and 6.0. Comparing this with Figure 7 we see that the number of iterations jumps from 3 to 2 at $t = 3.6$ and from 2 to 1 for $t = 6.0$. So there is a connection between an irregularity in the time convergence and a jump in the number of GMRES iterations to solve the momentum equations. This relation can also be observed for other choices of Re and Δt. To explain this phenomenon we note that in Figure 3 we plot

$$\frac{\rho_u^i}{1 - \rho_u^i} \frac{\|u^i - u^{i-1}\|_2}{\|u^i\|_2} \text{ with } \rho_u^i = \frac{\|u^i - u^{i-1}\|_2}{\|u^{i-1} - u^{i-2}\|_2}.$$

The quantity ρ_u^i is estimated by

$$\overline{\rho}_u^i = \frac{\|u_{n(i)}^i - u_{n(i-1)}^{i-1}\|_2}{\|u_{n(i-1)}^{i-1} - u_{n(i-2)}^{i-2}\|_2},$$

where $u_{n(i)}^i$ is the GMRES approximation of u^i. If $n(i) = n(i-1) - 1$, it is reasonable to expect that $\|u_{n(i)}^i - u^i\|_2$ is considerably larger than $\|u_{n(i-1)}^{i-1} - u^{i-1}\|_2$. This implies that $\overline{\rho}_u^i$ is a bad approximation of ρ_u^i if i is in the vicinity of a jump of $n(i)$.

3.3 A discussion of the termination criterion

We note that there should be a relation between ε_u and ε where ε is the required difference between the computed and the stationary solution as given in Section 2, e.g. it is necessary that ε_u is less than ε. Let us give some other open questions concerning the stopping criterion below:

- What is the influence of ε_u on the time convergence of the pressure correction method?

- Is it a good idea to choose ε_u as a function of n? A possibility could be: take ε_u^n relatively large for small n and small for large n, because for small n the exact solution has a large distance to the stationary solution, so it makes no sense to approximate the exact solution with an accurate solution of the discrete problem.

- From the foregoing it seems that the termination criterion: $\|r_j\|_2/\|r_0\|_2 \leq \varepsilon_u$, the relative precision of the residual with respect to the initial residual can be a good alternative. Advantages of this criterion: the number of iterations is approximately the same for every n (no minimum number of iterations required, and a good approximation of ρ_u and ρ_p), and the required accuracy varies with n in a natural way. Initially one has a bad initial guess and so the computed solution has a low accuracy, whereas after some time the starting solution becomes better and thus the computed solution has a high accuracy.

- The best criterion seems a combination: choose ε_{u1} larger that ε_{u2} and stop if $j < 10$ and $\|r_j\|_2 \leq \varepsilon_{u1}\|r_0\|_2 + \varepsilon_{u2}\|f^{n+1}\|_2$, or

$$\|r_j\|_2 \leq \varepsilon_{u1}\|r_0\|_2 + \varepsilon_{u2}\frac{\sigma_{10}^{(10)}}{\sigma_1^{(10)}}\|f^{n+1}\|_2.$$

3.4 Ritzvalues of the momentum equations

In this subsection we study the behaviour of the eigenvalues of M^n and discuss the consequences of this behaviour for the convergence of the linear solver and the convergence of the time integration.

We note that the momentum equations $M^{n+1}u^{n+1} = f^{n+1}$ comes from an Euler backward discretization of

$$\rho\frac{du}{dt} = \rho M(u)u.$$

So M^{n+1} can be written as $M^{n+1} = \frac{\rho}{\Delta t}I - \rho\overline{M}^{n+1}$, where the matrix $\overline{M}^{n+1}$ is an approximation of $M(u^{n+1})$. Using the GMRES method we calculate the eigenvalues of the Hessenberg matrix H_j (for definition of H_j see [11], p. 858), which are called Ritzvalues. These Ritzvalues are approximations of the eigenvalues of M^{n+1}. In general, there is a fast convergence to the extreme eigenvalues. So the convex hull of the calculated Ritzvalues gives a good approximation of the convex hull of the eigenvalues.

To obtain the Ritzvalues of M^{n+1} we solve the linear system without preconditioning. The Dirichlet boundary equations are included as an identity in the momentum equations. So we always get a Ritzvalue equal to one, which does not approximate an eigenvalue of $M(u^{n+1})$ (see [17], p. 9, 10). To get rid of this "wrong" Ritzvalue our startvector u_0^{n+1} is such that it satisfies the boundary conditions.

In the following figures we plot Ritzvalues of $\overline{M}^{n1}$, where $n1 = \frac{T}{\Delta t}$, for different choices of the Reynolds number Re, the timestep Δt, the space discretization and the endtime T. A Ritzvalue μ of $\overline{M}^n$ is obtained from a Ritzvalue λ of M^n using the relation

$$\mu = \frac{1}{\Delta t} - \frac{\lambda}{\rho}. \tag{5}$$

Accurate Ritzvalues are plotted with the symbol x, whereas inaccurate Ritzvalues are plotted with the symbol 0. In Figure 9 to 13 we choose $\Delta t = 0.125, T = 0.25$ and $Re = 1, 5, 10, 50, 100$($Re = 2\rho$ in these examples). Note that for $Re = 1$ all Ritzvalues are real, for $Re = 5, 10$ some Ritzvalues are complex, whereas for $Re = 50, 100$ nearly all Ritzvalues are complex. If Re increases the spectrum of $\overline{M}^2$ converges to the imaginary axis. In Table 3.1 we specify some additional information. In this table we specify the condition number of M^2, the maximal (minimal) real part of the Ritzvalues of $M^2 : \lambda_{max}(\lambda_{min})$, and the maximal (minimal) real part of the Ritzvalues of $\overline{M}^2 : \mu_{max}(\mu_{min})$. Note that an increase of Re leads to a decrease of the condition of M^2, and an increase of λ_{min}, μ_{max} and μ_{min}. We make the following observations with respect to the spectrum of M^2 and the convergence behaviour of GMRES: for $Re = 1, 5, 10$ the spectrum of M^2 is in the vicinity of the real axis. For increasing Re from 1 to 10 the ratio $\frac{\lambda_{max}}{\lambda_{min}}$ and the number of GMRES iterations decrease. For $Re = 50, 100$ the spectrum of M^2 has large imaginary components. The increase from $Re = 10$ to $Re = 100$ leads to an increase of the number of GMRES iterations.

Re	1	5	10	50	100
condition	255	91	51	12.5	7
λ_{max}	2296	2308	2310	2150	2200
λ_{min}	9	27	52	224	465
μ_{max}	-10	-2.9	-2.3	-0.95	-1.3
μ_{min}	-4585	-915	-454	-78	-36

Table 1: Properties for M^2 and $\overline{M}^2$ for $\Delta t = 0.125$.

In Figure 14 and 15 we plot results for $Re = 10, \Delta t = 0.125, T = 5$ and 10. Note that the Ritzvalues do not differ much, which agrees with the fact that this is a stationary problem, so $\overline{M}^{n+1} \to M(u)$ for n large enough. A consequence of this is that it is possible, that after some timesteps a fixed preconditioning saves some computing time.

In Figure 16, 11 and 17 we choose $Re = 10, \Delta t = 0.25, 0.125$, and 0.0625. As can be seen from the formula

$$M^n = \frac{\rho}{\Delta t} I - \rho \overline{M}^n \tag{6}$$

and the fact that $\overline{M}^n$ does not depend (much) on Δt it is expected that μ_{max} is constant for different choices of Δt, and thus λ_{min} is given by $\lambda_{min} = \frac{5}{\Delta t} - 5\mu_{max}$. Using $\mu_{max} = -2.3$ from Table 1 we obtain Table 2.

There is a good correspondence between the observed λ_{min} and the expected value of λ_{min}

Δt	0.25	0.125	0.0625
λ_{min}	31.5	52.0	89.0
λ_{exp}	31.6	51.5	91.5

Table 2: Dependence of λ_{min} on Δt.

given by λ_{exp}. From this we conclude that for n large enough the eigenvalues of M^n are only shifted along the real axis for different choices of Δt. This implies that if Δt decreases the eigenvalues of $\frac{\Delta t}{\rho} M^n$ cluster around 1, so the convergence of the GMRES method should be faster. This agrees with our observations given in Figure 8.

In Figure 18 we show the Ritzvalues for $Re = 10, \Delta t = 0.125$ and $T = 5$ on an 8×32 grid. From this it seems that the imaginary part of the convex hull of M^n grows like $O(\frac{1}{h})$ and $|\mu_{min}|$ grows as $O(\frac{1}{h^2})$ for decreasing h.

Conclusions

In this subsection we have calculated Ritzvalues (approximate eigenvalues) of $\overline{M}^n$, and indicated how the Ritzvalues depend on $Re, \Delta t$ and the space discretization. This dependence agrees with practical and theoretical results known for the eigenvalues of the momentum equations. This increases our confidence in the correctness of the discretized momentum equations. Furthermore, the Ritzvalues give useful information to understand and predict the convergence behaviour of the iterative solution method (GMRES).

3.5 The time integration and Ritzvalues

In this subsection we give an application of the Ritzvalues with respect to the convergence of the time integration. We solve a small test problem, which has a large jump in the finite volumes in the x_1-direction. The mesh of this problem is given in Figure 19. Starting with $u^0 = 0$ we try to calculate the stationary solution $u = 1$. We observe that for large $\Delta t (\Delta t = 0.1)$ the time integration converges, whereas for small $\Delta t (\Delta t = 0.01)$ the time integration diverges.

To understand this strange behaviour we calculate the Ritzvalues of $\overline{M}^n$, which are given by: -11.7, -11.2, -1.64 $\pm 3.2i, -1.58 \pm 3.2i, -1.4 \pm 3.2i, -0.56, -0.18, 33.1, 33.5$.Note that some Ritzvalues of $\overline{M}^n$ positive. This indicates that the discretization of the momentum equations is incorrect, since we expect that the real parts of the eigenvalues are negative. Furthermore, this enables us to understand that the choice $\Delta t = 0.1$ leads to convergence, whereas $\Delta t = 0.01$ leads to divergence. It is known that Euler backward applied to $\frac{du}{dt} = \beta u$ has as stability region $|1 - \beta \Delta t| > 1$. This implies that only Ritzvalues with a positive real part can cause instability. For Ritzvalues 33.1 and 33.5 and $\Delta t = 0.1$ we obtain $33.1 \times 0.1 = 3.31$ and $33.5 \times 0.1 = 3.35$ and so Euler backward is stable, whereas $\Delta t = 0.01$ gives $33.1 \times 0.01 = 0.331$ and $33.5 \times 0.01 = 0.335$ and Euler backward is instable. This agrees with our observations.

Our research shows that in this case the finite volume discretization described in [13] is not stable for large jumps in the meshes, and hence can only be applied for relatively small ratios in gridsize. In fact our testproblem motivates a subject of further study: to construct a discretization such that eigenvalues of the discretized momentum equations with a positive real part are avoided, also if there is a (large) jump in the finite volume mesh.

4 The pressure equation

The pressure equation is solved with a variant of the GMRES method. In this new method, named the GMRESR(m) method (see [14], [17], and [18]), we take a different preconditioner in each iteration. As preconditioner we choose m steps of GMRES. In this section we consider the following termination criteria, which can be combined with an iterative solution method, e.g. GMRESR: stop the iterative solution method if

- the ratio of the norm of the final and initial residual is less than a given accuracy, or
- the estimated norm of the relative error is small, or
- the norm of the divergence of the velocity is small enough.

Until now the solution of the pressure equation is the most time-consuming part. So it is important to have a good termination criterion, which means that the accuracy of the final iterate is sufficient, whereas the number of required iterations is as small as possible. We illustrate the stopping strategies by some numerical experiments.

The residual criterion

To obtain an approximation of the pressure p^{n+1} we solve the linear system

$$P\Delta p^{n+1} = g^{n+1}, \tag{7}$$

where Δp^{n+1} is an approximation of $p^{n+1} - p^n$. We start with $\Delta p_0^{n+1} = 0$ and stop if the inequality

$$\frac{\|g^{n+1} - P\Delta p_j^{n+1}\|_2}{\|g^{n+1}\|2} \leq \varepsilon_p \tag{8}$$

holds, where ε_p is a given quantity. Note that the linear system originates from a discretization of the following equation [17]; equation (5):

$$\frac{\partial^2(p^{n+1} - p^n)}{\partial x_1^2} + \frac{\partial^2(p^{n+1} - p^n)}{\partial x_2^2} = \frac{1}{\Delta t}\left(\frac{\partial \hat{u}_1^{n+1}}{\partial x_1} + \frac{\partial \hat{u}_2^{n+1}}{\partial x_2}\right). \tag{9}$$

Since $\hat{u}^{n+1} \to u$, $n \to \infty$ and $div\ u = 0$ we expect and observe that $\|div\ \hat{u}^{n+1}\|_2 \to 0$. Using the given stop criterion, this implies that the required accuracy of $p^{n+1} - p^n$ grows considerably. This can be a disadvantage, suppose that $\|div\ \hat{u}^{n+1}\|_2 \simeq 10^{-15}$ and $\|u^{n+1}\|_2 \simeq 1$ then GMRESR stops if

$$\|g^{n+1} - P\Delta p_j^{n+1}\|_2 \leq \varepsilon_p \cdot 10^{-15}.$$

However due to rounding errors (using a computer with a relative machine precision equal to 10^{-15}) we obtain that $\|div\ u^{n+1}\|_2/\|u^{n+1}\|_2 \simeq 10^{-15}$. In such a case the solution of the pressure equation is a waste of computing time.

The error criterion

To overcome the above mentioned disadvantage we can use the following termination criterion: stop if the inequality

$$\frac{\|\Delta p^{n+1} - \Delta p_j^{n+1}\|_2}{\|p^{n+1}\|_2} \leq \varepsilon_p, \tag{10}$$

holds. Using this termination criterion we are able to obtain an idea of the error in the pressure. Since the exact solution Δp^{n+1} is not known we use the following stopping strategy. In the first timestep we compute $1/\sigma_{10}^{(10)}$ (as for the momentum equations), which is an approximation of $\|P^{-1}\|_2$, and stop if

$$\|g^{n+1} - P\Delta p_j^{n+1}\|_2 \leq \sigma_{10}^{(10)}\|p^n\|_2\, \varepsilon_p.$$

This termination criterion implies that

$$\frac{\|\Delta p^{n+1} - \Delta p_j^{n+1}\|_2}{\|p^{n+1}\|_2} \leq \|P^{-1}\|_2 \frac{\|g^{n+1} - P\Delta p_j^{n+1}\|_2}{\|p^{n+1}\|_2} \simeq \frac{1}{\sigma_{10}^{(10)}} \frac{\|g^{n+1} - P\Delta p_j^{n+1}\|_2}{\|p^n\|_2} \leq \varepsilon_p.$$

The divergence criterion

A third idea is to stop if the $\|div\ u^{n+1}\|_2$ is small enough. To achieve this, we note that ([17]; equation (5))

$$u_i^{n+1} = \hat{u}_i^{n+1} + \Delta t \frac{\partial(p^n - p^{n+1})}{\partial x_i}, \quad i = 1, 2,$$

and thus

$$div\ u^{n+1} = \frac{\partial \hat{u}_1^{n+1}}{\partial x_1} + \frac{\partial \hat{u}_2^{n+1}}{\partial x_2} + \Delta t \left\{ \frac{\partial^2(p^n - p^{n+1})}{\partial x_1^2} + \frac{\partial^2(p^n - p^{n+1})}{\partial x_2^2} \right\}.$$

Comparing this with equation (7) and (8) we observe that

$$\|div\ u^{n+1}\|_2 = \Delta t\ \|g^{n+1} - P\Delta p_j^{n+1}\|_2.$$

This implies that if we stop when

$$\|g^{n+1} - P\Delta p_j^{n+1}\|_2 \leq \frac{\|u^n\|_2}{\Delta t}\, \varepsilon_{div} \tag{11}$$

then $\frac{\|div\ u^{n+1}\|_2}{\|u^{n+1}\|_2} \leq \varepsilon_{div}$.

Note that the norm of the residual approximates $\|div\ u^{n+1}\|_2$. In this respect GMRES has the advantage that it computes the residual with minimal norm in the current Krylov subspace. It is possible to precondition the pressure equation in order to obtain a fast convergence.

However, this implies that the relation between the residual and the $div\ u^{n+1}$ is lost. So if we use this termination criterion it is better to postcondition the pressure equation.

In depends on the problem which criterion should be used. Use (10) as a stop criterion in order to obtain an accurate approximation of the pressure. On the other hand if one wants a small norm of $div\ u^{n+1}$, (11) is the best choice. A combination of (8) and (11) seems a good idea too, because initially it is not necessary to have a small norm of $div\ u^{n+1}$, it is only necessary to compute the pressure (satisfying (8)) such that pressure correction scheme converges. Only in the final time step(s) it is necessary to use condition (11). A possibility to achieve this: ($r_j := g^{n+1} - P\Delta p_j^{n+1}$) stop if $\|r_j\|_2 \leq \max(\varepsilon_p \|r_0\|_2,\ \varepsilon_{div} \frac{\|u^n\|_2}{\Delta t}), n \leq N_t - 2$, and stop if $\|r_j\|_2 \leq \varepsilon_{div} \frac{\|u^n\|_2}{\Delta t}$ in the final timestep ($n = N_t - 1$).

We use the start solution $\Delta p_0^{n+1} = 0$ because we expect that $\|\Delta p^{n+1}\|_2 = 0(\Delta t)$ is small. Note that Δp_j^n approximates $\Delta t \frac{dp^n}{dt}$. If p is a slowly varying function of t then Δp_j^n is also a good approximation of $\Delta t \frac{dp^{n+1}}{dt}$. This motivates us to use the startvector $\Delta p_0^{n+1} = \Delta p_j^n$. In our numerical experiments the choice $\Delta p_0^{n+1} = \Delta p_j^n$ gives slightly better results than the choice $\Delta p_0^{n+1} = 0$.

An open question is: what are the relations between the termination criteria given in this section, the termination criteria for the momentum equations and the convergence behaviour and termination criteria of the time integration.

Numerical experiments

In [14] it is shown that an optimal choice of m in the GMRESR(m) method is given by $m = \sqrt[3]{3mg}$, where m_g is the number of full GMRES iterations. Since $m_g \geq 180$ in this problem (see [17]; p.6) we use GMRESR(10) to solve the pressure equation. Since we do not use a preconditioner the residual is related to $div\ u^{n+1}$. In our experiments we choose $Re = 10, \Delta t = 0.125$ and $T = 5$ (40 timesteps). The results are given in Table 3.

Experiment 1

Our usual choices are to stop if $\|r_k\|_2 \leq 10^{-6} \|r_0\|_2$ and start with $\Delta p_0^{n+1} = 0$.

Experiment 2

In order to compare a different choice of the start vector, we solve the pressure equation with $\Delta p_0^{n+1} = 0$ and termination criterion $\|r_k\|_2 \leq 10^{-9}$.

Experiment 3

We take the same termination criterion $\|r_k\|_2 \leq 10^{-9}$ but start with $\Delta p_0^{n+1} = \alpha \Delta p_j^n$ where α is such that $\|r_0\|_2$ is minimal.

In the following experiments we stop the GMRESR iteration if $\|r_k\|_2 \leq \varepsilon_1 + \varepsilon_2\ \|r_0\|_2$ with $\varepsilon_1 = \varepsilon_{div} \frac{\|u^n\|_2}{\Delta t}$.

Experiment 4

Start vector $\Delta p_0^{n+1} = 0$, $\varepsilon_{div} = 10^{-6}$, and $\varepsilon_2 = 10^{-6}$.

Experiment 5
Start vector $\Delta p_0^{n+1} = \alpha \Delta p_j^n$, $\varepsilon_{div} = 10^{-6}$, and $\varepsilon_2 = 10^{-6}$.

Experiment 6
Start vector $\Delta p_0^{n+1} = \alpha \Delta p_n^n$, $\varepsilon_{div} = 10^{-6}$, and $\varepsilon_2 = 10^{-3}$.

experiment	1	2	3	4	5	6	7
CPU (total)	49	50	46	36	32	28	17
pressure CPU	36	38	34	24	20	16	4.8
pressure iterations	688	732	667	468	395	323	466
momentum CPU	4	4	4	4	4	4	4
momentum iterations	149	149	149	149	149	149	149

Table 3: Total CPU times and iterations after 40 timesteps

Experiment 7
Combining the solution strategy of Experiment 6 with full GMRES and a post conditioning, we obtain the results given in Table 3. As MILU postconditioner we take an incomplete decomposition $LU = A - R$, where L and U have the same non-zero structure as the pressure matrix P. To obtain L and U we require that $(LU)_{ij} = P_{ij}$ if $i \neq j$ and $P_{ij} \neq 0, L_{ii} = 1$ and U_{ii} is such that $\sum\limits_i (LU)_{ij} = \sum\limits_i P_{ij}$.
We observe that the computed solutions at $t = 5$ are more or less the same in every experiment. This means that a good termination criterion saves CPU time. Comparing Experiment 1 and 6 we observe that the amount of iterations and computing time to solve the pressure equation is halved. Comparing Experiment 6 and 7 we note that one GMRESR(10) iteration costs 10 matrix vectorproducts. This explains the observation that the amount of pressure iterations in Experiment 6 is less than the amount in Experiment 7, but the CPU-time in Experiment 6 is much more than the CPU-time used in Experiment 7. Note that in Experiment 7 the solution of the pressure equation costs 28% of the total CPU-time, whereas the construction of the momentum equations costs 48% of the total CPU-time.

Conclusions

In this section we discuss some termination strategies for the pressure equation. One of our termination criteria relates the accuracy of the pressure solution with the divergence of the resulting velocity field. This relation only holds if the pressure equation is not preconditioned (postconditioning is allowed). Thereafter we give some choices of startvectors for the iterative solution method. We end the section with some numerical experiments. From these experiments it appears that the solution strategy given in Experiment 7 is superior to the strategies given in the other experiments.

5 The transport equation

In this section we give a short description of a transport equation. Such an equation can be used to describe the transport of temperature, certain quantities occuring in engineering models of turbulence, the concentration of salt in an estuary, etc. The property, which is transported, is denoted by c, which is a function of the space- and time variable. The function c satisfies the following convection-diffusion equation (in Cartesian coordinates):

$$\frac{\partial c}{\partial t} + k_1 u_1 \frac{\partial c}{\partial x_1} + k_2 u_2 \frac{\partial c}{\partial x_2} c - \left(k_3 \frac{\partial^2 c}{\partial x_1^2} + k_4 \frac{\partial^2 c}{\partial x_2^2} \right) = 0,$$

where $k_i,\ i = 1, 2, 3, 4$ are given functions. Furthermore, c satisfies given initial and boundary conditions.

There are several different applications using a transport equation. Firstly we consider the transport of a so-called passive scalar. In this case the Navier-Stokes equations can be solved independently of the transport equation. Thereafter u_1 and u_2 can be used to solve the transport equation. Secondly, there are applications where the Navier-Stokes equations are coupled with the transport equation(s), e.g., the Boussinesque problem ([12]; p.30) or turbulence modelling [3] (transport of an active scalar).

The discretization of the transport equation in general coordinates is analogous to the discretization of the momentum equations, which is described in the introduction (for further details see [4] and [13]). The discretization leads to the following linear system of equations:

$$C^{n+1} c^{n+1} = d^{n+1}.$$

The structure of the transport matrix C^{n+1} is the same as the structure of the pressure matrix P (see [17]; Figure 2). As an iterative method we use GMRES. It appears that the convergence properties of GMRES applied to the transport equation resembles the properties of GMRES applied to the momentum equations. This corresponds with the fact that the transport equation looks like the momentum equations. Using this resemblance we suggest to take as starting vector the solution of the foregoing time-step: $c_0^{n+1} = c_j^n$. Furthermore we use the following stopping strategy ($r_j = d^{n+1} - C^{n+1} c_j^{n+1}$): choose ε_{c1} larger than ε_{c2} and stop if $i < 10$ and $\|r_i\|_2 \leq \varepsilon_{c1} \|r_0\|_2 + \varepsilon_{c2} \|d^{n+1}\|_2$ or $\|r_i\|_2 \leq \varepsilon_{c1} \|r_0\|_2 + \varepsilon_{c2} \frac{\sigma_{10}^{(10)}}{\sigma_1^{(10)}} \|d^{n+1}\|_2$, which is the same strategy as we use for the momentum equations.

As usual there remain some open questions. Firstly, how should one choose the timestep Δt? Is it possible to use different timesteps for the momentum equations and the transport equations? Or to change the timestep as a function of the time t. If the Navier-Stokes equations and the transport equation(s) are coupled, what is the relation between the stop criteria in the time integration, the momentum-, the pressure- and the transport equations?

Conclusions

We analyse starting and stopping strategies for the transport equation. It appears that the structure of the discretized transport equation is the same as the discretized pressure equation, whereas the convergence behaviour of the iterative method applied to the transport equation is comparabe with the momentum equations. This motivates us to propose the same type of start vector and termination criterion as for the momentum equations.

6 Conclusions

In this paper we have discussed some strategies to solve the discretized incompressible Navier-Stokes equations. We have restricted ourselves to equations which have a stationary solution. In every section we have proposed topics for further research.

Time integration

In Section 2 we have specified a termination criterion for the time integration. This criterion is valid if the inequalities $\rho_u^n \leq \rho_u < 1$ hold. We have shown how to check these conditions in practice. If these inequalities are not satisfied, the behaviour of ρ_u^n can be used to analyse (and enhance) the time integration.

Momentum equations

In Section 3 we have discussed termination criteria for the momentum equations. The influence of different starting vectors, Δt, and required accuracy on the convergence behaviour of the iterative method are analysed and illustrated with numerical experiments. These insights lead us to an optimal termination criteria (Section 3.3). Next, we have calculated Ritzvalues (approximate eigenvalues) for the momentum equations and compared these with the convergence of the iterative solution method and the time integration.

Pressure equation

In Section 4, a new starting vector has been given for the pressure equation. Furthermore we have discussed three termination criteria. One of these criteria relates the accuracy of the pressure solution to the divergence of the resulting velocity field. From numerical expirements we have noted that we gain a considerable amount of CPU time, using the new starting vector and termination criterion.

Transport equation

Finally, in Section 5 we have given starting and stopping strategies for the transport equation.

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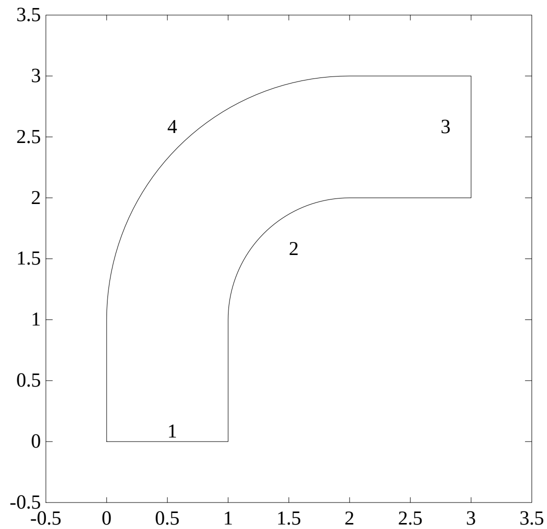

Figure 1: The physical domain of the test problem

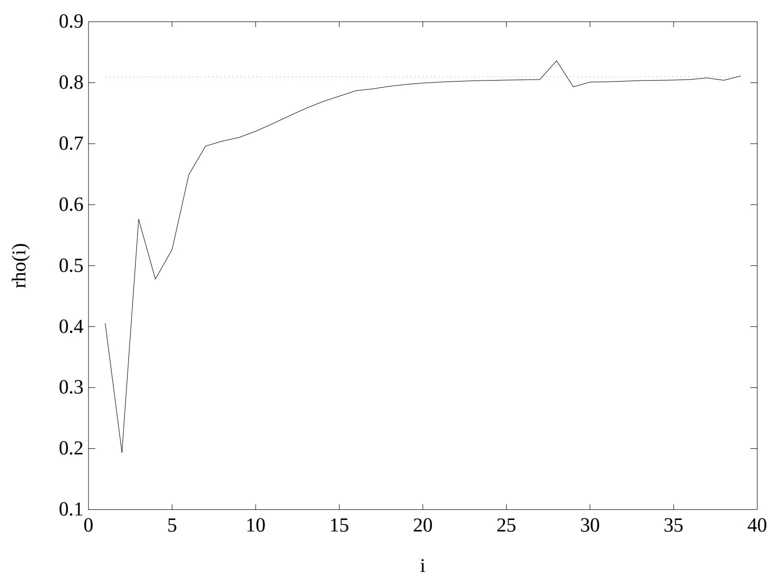

Figure 2: The quantity $\frac{||u^i - u^{i-1}||_2}{||u^{i-1} - u^{i-2}||_2}$ for $Re = 10$ and $\Delta t = 0.0625$

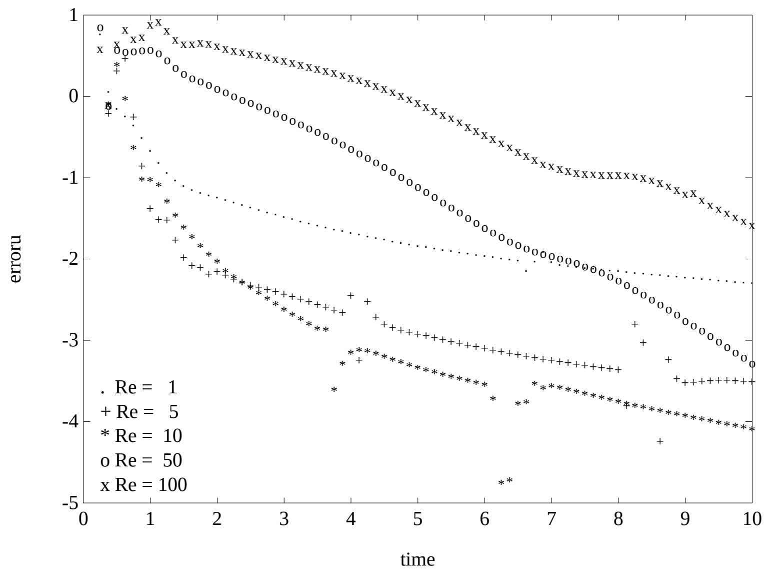

Figure 3: The estimated error in the velocity, $\Delta t = 0.125$

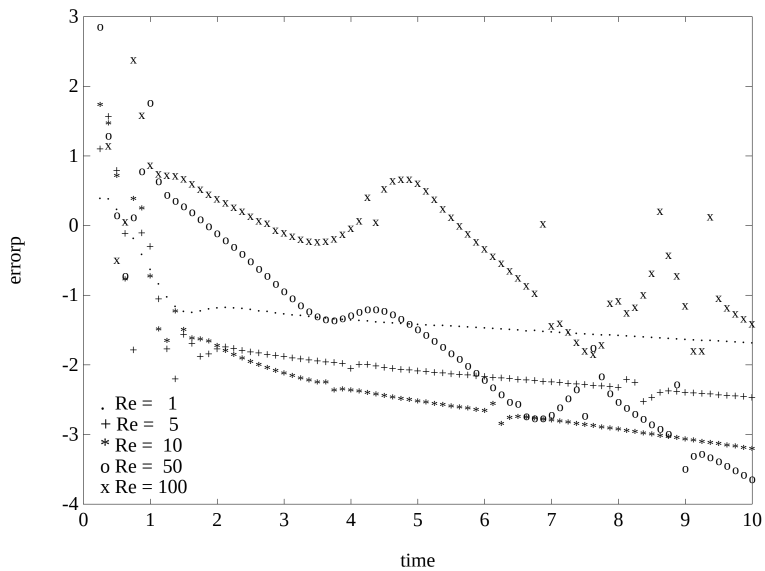

Figure 4: The estimated error in the pressure, $\Delta t = 0.125$

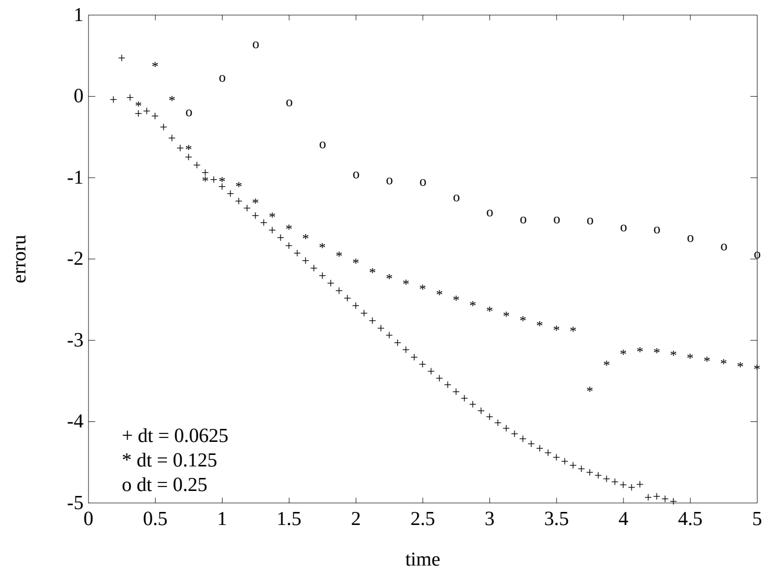

Figure 5: The estimated error in the velocity, $Re = 10$

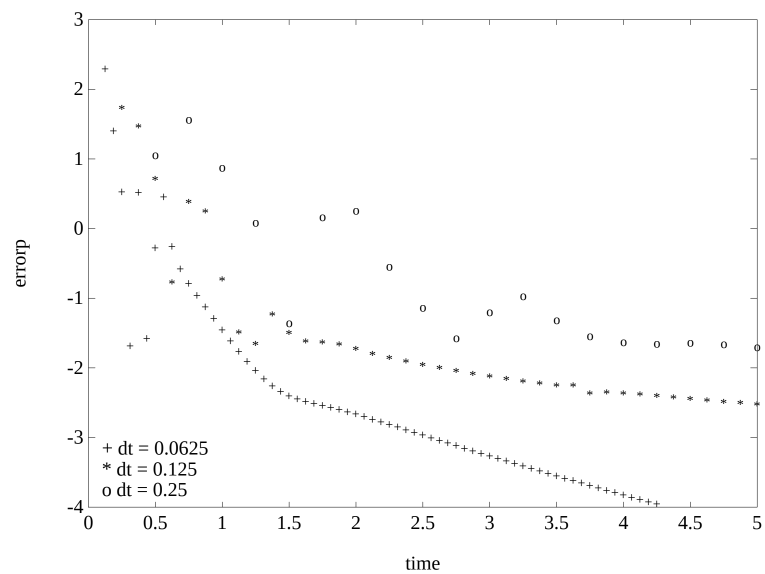

Figure 6: The estimated error in the pressure, $Re = 10$

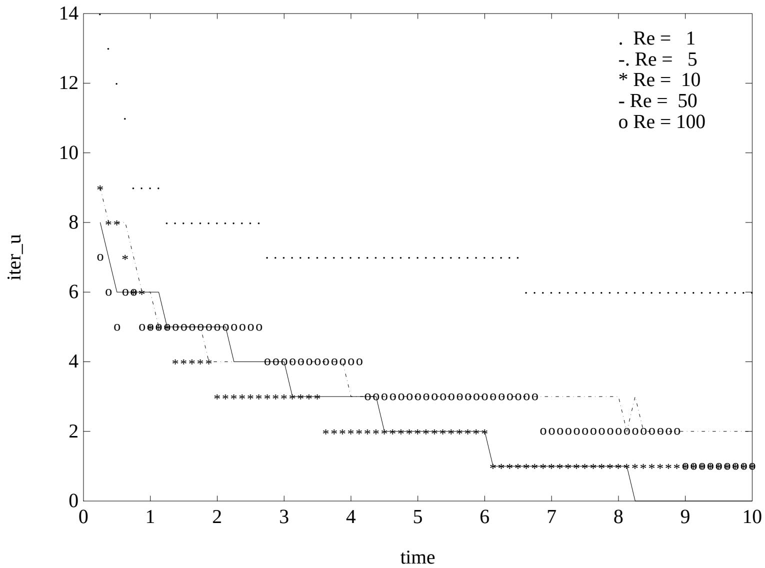

Figure 7: Number of GMRES iterations to solve the momentum equations $\Delta t = 0.125$

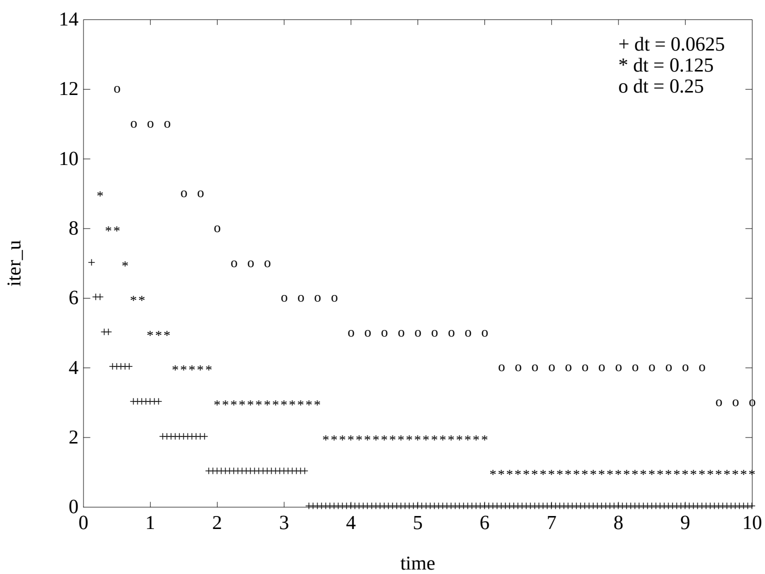

Figure 8: Number of GMRES iterations to solve the momentum equations, $Re = 10$

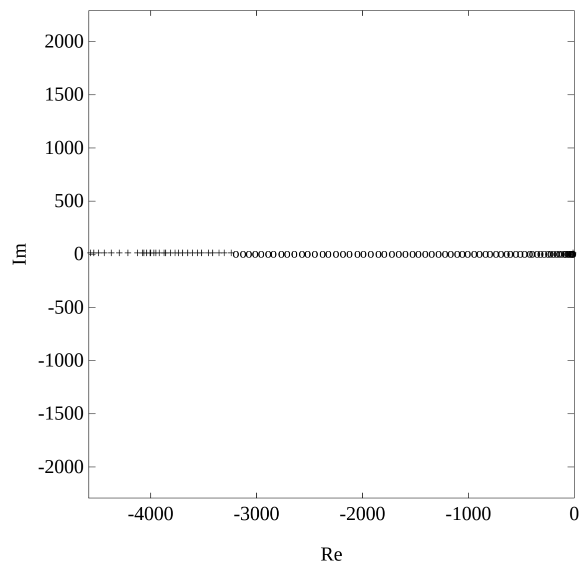

Figure 9: Ritzvalues of $\overline{M}^2, Re = 1, \rho = 0.5, \Delta t = 0.125$

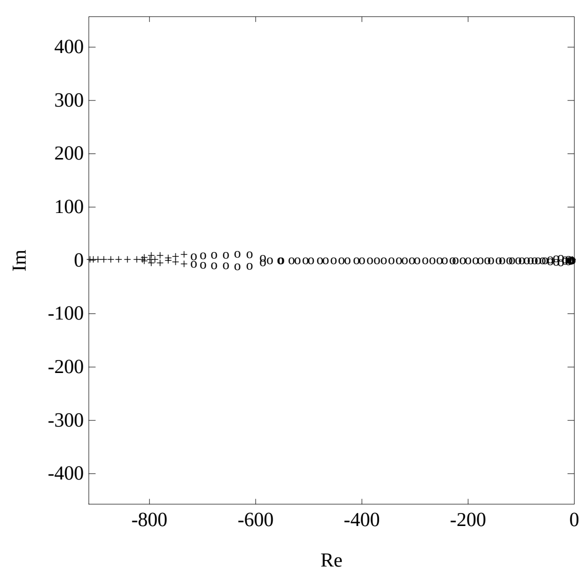

Figure 10: Ritzvalues of $\overline{M}^2, Re = 5, \rho = 2.5, \Delta t = 0.125$

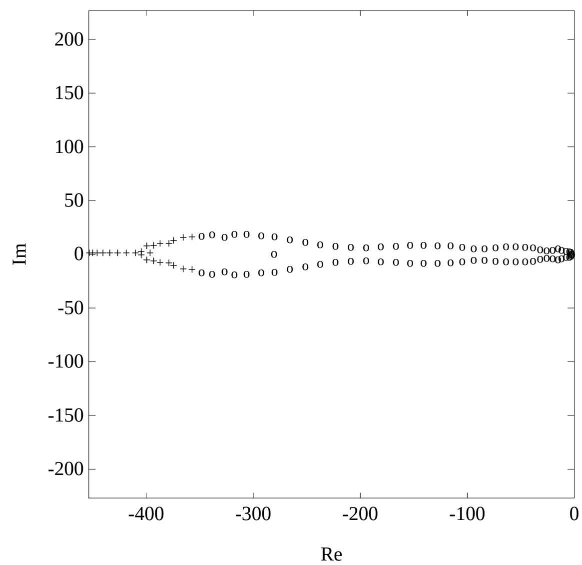

Figure 11: Ritzvalues of $\overline{M}^2, Re = 10, \rho = 5, \Delta t = 0.125$

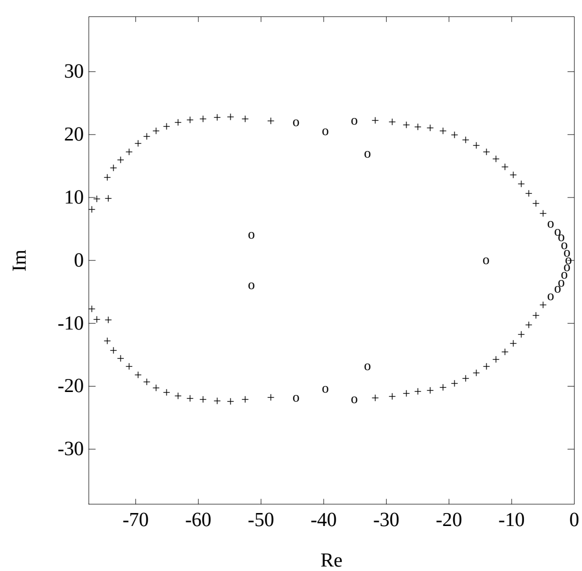

Figure 12: Ritzvalues of $\overline{M}^2, Re = 50, \rho = 25, \Delta t = 0.125$

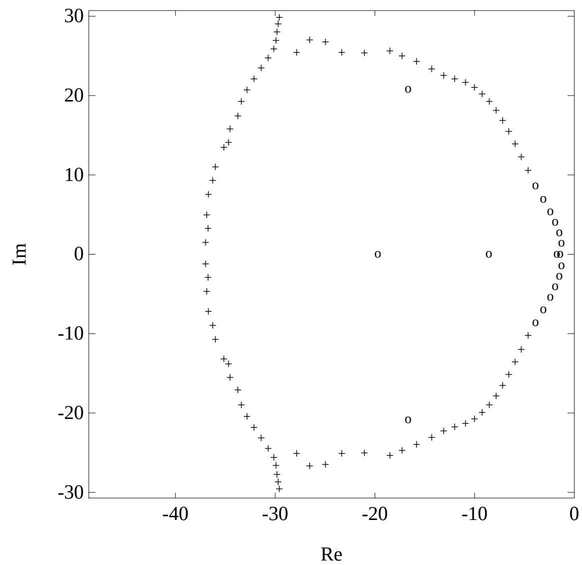

Figure 13: Ritzvalues of $\overline{M}^2, Re = 100, \rho = 50, \Delta t = 0.125$

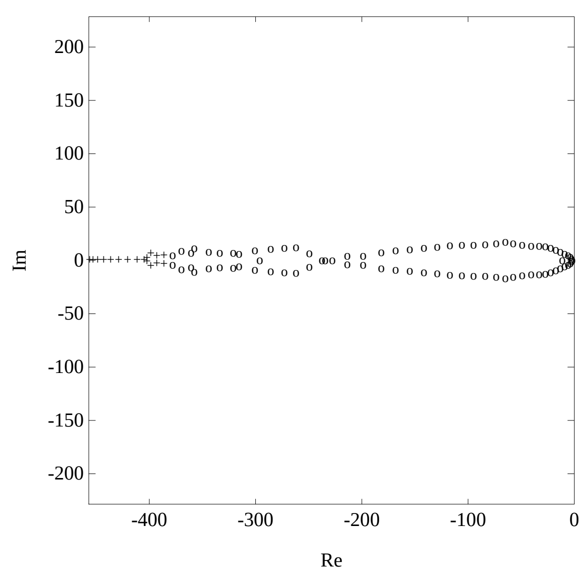

Figure 14: Ritzvalues of $\overline{M}^{40}, Re = 10, \rho = 5, \Delta t = 0.125$

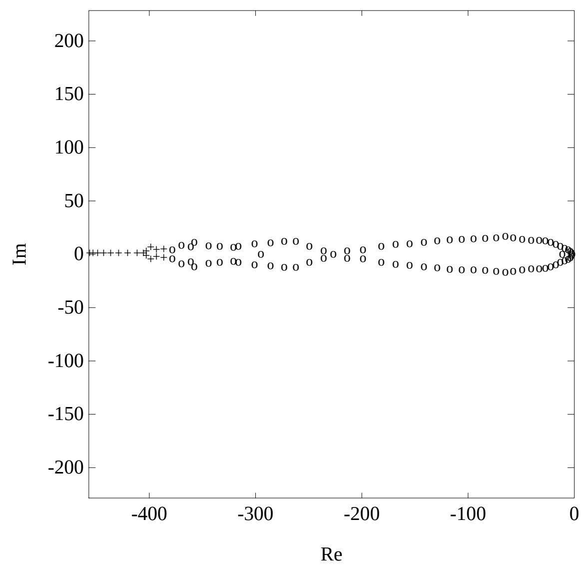

Figure 15: Ritzvalues of $\overline{M}^{80}, Re = 10, \rho = 5, \Delta t = 0.125$

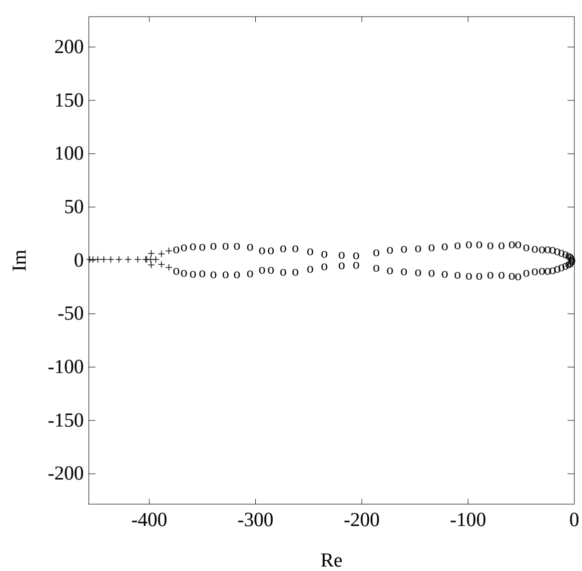

Figure 16: Ritzvalues of $\overline{M}^{2}, Re = 10, \rho = 5, \Delta t = 0.25$

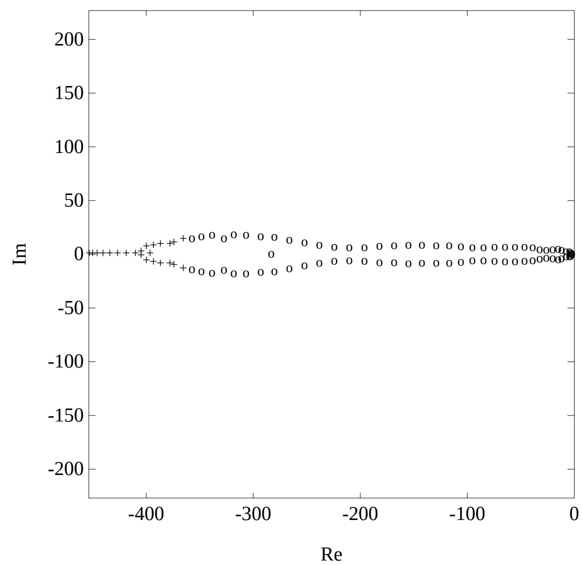

Figure 17: Ritzvalues of $\overline{M}^4, Re = 10, \rho = 5, \Delta t = 0.0625$

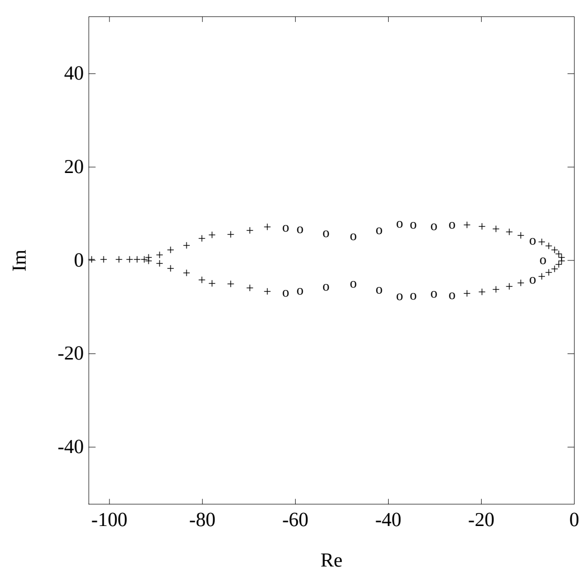

Figure 18: Ritzvalues of $\overline{M}^{40}, Re = 10, \rho = 5, \Delta t = 0.125$, and 8×32 finite volumes

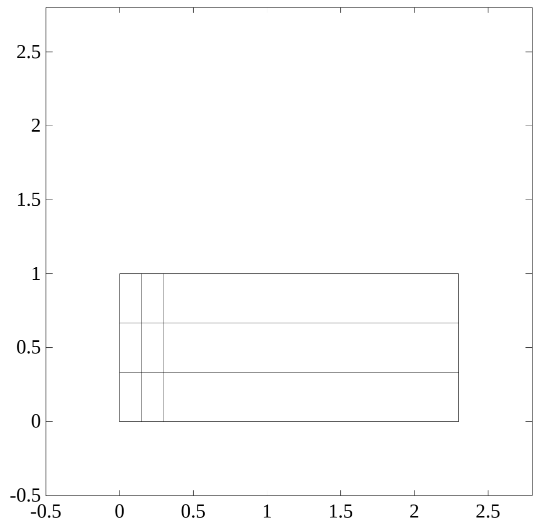

Figure 19: Mesh used in our small testproblem