Internship Report

Fractional Step Methods for Incompressible Flow

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Preface and Acknowledgement

This report is part of my internship at the Department of Computer Applications in Science and Engineering in Barcelona Supercomputing center (BSC) for a period of 3 months. BSC specializes in High Performance Computing and manages Marenostrum, one of the most powerful supercomputers in Europe. This internship was a part of my 2 year masters program in Computational Mechanics at UPC, Barcelona.

I worked on the Fractional Step Methods for Navier Stokes equations in Incompressible flow. Through this internship, I not only had the opportunity to gain a lot of knowledge, but more importantly, I also had the chance to sharpen my skills in a professional working environment.

I would like to express my gratitude to Mr. Guillaume Houzeux for giving me this opportunity at BSC. He was my mentor and gave me valuable instructions and directions throughout the internship. I would also like to thank Mr. Oriol Lehmkuhl for all the in-time feedback and guidance provided. In short, I would like to thank BSC and CIMNE, UPC from providing me this great opportunity in which I have developed academically, professionally and socially.

Introduction

A major difficulty in the numerical simulation of the Incompressible Navier-Stokes equation is that the Velocity and Pressure are coupled through the incompressibility constraint. Pressure is an implicit variable which instantaneously adjusts itself in such a way that the velocity remains divergence free. The most attractive feature of Fractional Step Methods is that, at each time step, one only needs to solve a sequence of decoupled elliptic equations for the velocity and pressure, making it very efficient for large scale numerical simulations.

Fractional step methods consist of Standard, Incremental and Rotational forms of Pressure and Velocity correction methods. Pressure correction methods consist of a basic predictor – corrector procedure between pressure and velocity fields. Using an initial approximation of the pressure, the momentum equation can be solved to obtain an intermediate velocity field. This velocity, in general, does not satisfy the divergence-free constrain and must therefore be corrected. By taking the divergence of the momentum equation and enforcing the incompressibility constraint, a Poisson equation for the pressure is obtained. Solving this equation for pressure, the final velocity can then be obtained.

Governing Equation

Consider an open and bounded domain **Ω** with boundary **Γ** for t ≥ 0. Since the non-linear term in the Navier Stokes equations does not affect the convergence rate, it is omitted and the time dependent Stokes equations given below is considered.

$$\begin{aligned}
&\partial_t \mathsf{u} - \nu\nabla^2\mathsf{u} + \nabla\mathsf{p} = f \quad \text{in } \Omega\times[0,T],\\
&\nabla\cdot\mathsf{u} = 0 \quad \text{in } \Omega\times[0,T],\\
&\mathsf{u}|_\Gamma = 0 \quad \text{in } [0,\mathrm{T}], \qquad \text{and } \mathsf{u}|_{t=0} = u_0 \quad \text{in } \Omega,
\end{aligned}$$

where u(*x,t)* is the velocity vector, *p(x,t)* is the kinematic pressure, *f*(*x,t)* is the body force vector and ν is the kinematic viscosity. Homogeneous Dirichlet boundary condition is considered for velocity for the sake of simplicity.

Pressure Correction Schemes

Pressure-correction schemes are time-marching techniques composed of two sub-steps for each time step: the pressure is treated explicitly or ignored in the first sub-step and is corrected in the second one by projecting the provisional velocity onto the Divergence free space.

Non – Incremental Explicit Pressure Correction Scheme (Standard Form)

There is a lot of Literature available on the Implicit form of the Non-Incremental pressure correction scheme, however, the explicit form was implemented in Alya, a Computational Mechanics simulation code developed at BSC as it has lower computational time compared to the implicit method.

For the Explicit Euler time stepping method, Pressure is ignored in the first sub step and the intermediate velocity $\hat{u}$ is found from the explicit equation

$$\frac{\hat{u}^{k+1}}{\Delta t} = \frac{u^k}{\Delta t} + f^{k+1} + \nu \nabla^2 \hat{u}^{k+1} \quad (1)$$

The pressure is corrected in the second sub step by projecting the intermediate velocity into the divergence free space, to get the pressure Poisson equation given by :

$$\Delta t \nabla^2 p^{k+1} = \hat{u}^{k+1} \quad (2)$$

Finally, the end of step velocity is found as,

$$u^{k+1} = \hat{u}^{k+1} - \Delta t \nabla p^{k+1} \quad (3)$$

The stability of the scheme depends on the time step Δt . The time step size cannot be greater than the critical time step for the Explicit method. However, Δt also determines the pressure stability and hence cannot be much lesser than the critical time step.

It is observed that the boundary condition $\nabla p^{k+1}.n = 0$ is enforced at the boundaries on the pressure. This artificial boundary condition induces a numerical boundary layer that prevents the scheme from being fully first order on the velocity in the H1 norm and on the pressure in the L2 norm.

Explicit Rotational Pressure Correction Scheme

To overcome the problem of artificial boundary condition, the Pressure in the step 2 is replaced by a pressure like term given by

$$\phi^{k+1} = p^{k+1} + \nu \nabla . \hat{u}^{k+1}$$

This change enforces a consistent boundary condition on Pressure.

The end of step velocity is now given by:

$$u^{k+1} = \hat{u}^{k+1} - \Delta t \nabla \phi^{k+1}$$

These two schemes were implemented as FORTRAN code in Alya. The details of the implementation cannot be provided as it is property of BSC. The code verification was done using the Method of Manufactured Solutions (MMS).

Method of Manufactured Solution

A manufactured solution is an exact solution to some PDE or set of PDE’s that has been constructed by solving the problem backwards. Using the manufactured solution the source term of the PDE is evaluated. Now, the solution to the PDE with this source term is found to evaluate the error.

To compute the discretization error, several measures are possible. The normalized L2 norm error is given by

$$e_2 = \sqrt{\frac{1}{N} \sum_n (u_n - U_n)^2}$$

where u_n is the manufactured solution evaluated at n and U_n is the discrete solution. The normalized L1 error is given by

$$e_1 \quad = \quad \frac{1}{N}\sum_n (u_n - U_n)$$

Similarly, the infinity norm of the global error is given by

$$e_\infty \quad = \quad max_n(u_n - U_n)$$

In the tables below W(,1) denotes the L1 norm, W(,2) denotes the L2 norm and W(,i) denotes the infinity norm. These values for the primary variable are denoted by W(0,) and for the gradient of the primary variable by W(1,).

Mesh and Time Convergence Analysis using MMS

Results for the Mesh and Time convergence analysis for the Explicit non-incremental pressure correction method are given below. The domain is a cubical cavity of unit size along each dimension. The original mesh has 1000 hexahedral elements. Second order interpolation was used for both Velocity and Pressure.

For the explicit method, the Courant Friedrichs Lewy (CFL) condition (which relates the time step size to the element size) of value 1 is used. Hence it is difficult to isolate the spacial errors or temporal errors. Changing the element size changes the critical time step and the resulting global error is a combination of both temporal and spacial errors.

Mesh Convergence

The mesh convergence is done by dividing each element in the mesh and then finding the global error for the refined mesh. The divided element has half the dimensions of the original element.

Time integration using 2nd order Adam Bashforth method for the time derivative term. Critical time step was used.

1. Using Quadratic Solution

u = (1.0 + x + y^2+z^2)
v = -(1.0 + y + x^2 + z^2)
w = (x^2 + y^2)

p = 2x + 3y

No mesh division

Norm	Velocity Error	Pressure Error
W(0,1)	2.00E-03	6.37E-02
W(0,2)	1.78E-03	6.34E-02
W(0,i)	1.02E-03	1.72E-01
W(1,1)	4.35E-02	1.87E-01
W(1,2)	4.47E-02	2.79E-01
W(1,i)	3.32E-02	8.47E-01

Division = 1

Norm	Velocity Error	Pressure Error	Velocity Order	Pressure Order
W(0,1)	5.00E-04	1.78E-02	1.9997691411	1.8427966648
W(0,2)	4.45E-04	1.80E-02	2.0002432123	1.8212921262
W(0,i)	2.57E-04	8.74E-02	1.9933549976	0.9735815839
W(1,1)	2.17E-02	9.00E-02	1.0039146899	1.0512420941
W(1,2)	2.24E-02	1.83E-01	1.0001290194	0.6039138758
W(1,i)	1.66E-02	8.40E-01	1.0040038621	0.0128982452

Division = 2

Norm	Velocity Error	Pressure Error	Velocity Order	Pressure Order
W(0,1)	1.25E-04	4.80E-03	1.999942291	1.8891009837
W(0,2)	1.11E-04	4.94E-03	2.0001621643	1.862335775
W(0,i)	6.44E-05	4.41E-02	1.9950418562	0.9867246804
W(1,1)	1.08E-02	4.39E-02	1.0022607569	1.0352834082
W(1,2)	1.12E-02	1.24E-01	1.000064514	0.5636305256
W(1,i)	8.27E-03	8.38E-01	1.0012207756	0.0035785242

It is seen that Velocity and Pressure have second order of spacial convergence for the L2 norm which verifies the code for Explicit non-incremental pressure correction method. Another exact solution – Taylor Green Vortex is used for a square cavity of unit size along each dimension as shown below.

2. Taylor Green Vortex

u = - cos(x) sin(y) f(t)
v = sin(x) cos(y) f(t)

where f(t) = exp(-2 pi^2 t)

p = - 0.25 (cos(2x) + cos (2y)) f(t)^2

No mesh Divisions

Norm	Velocity Error	Pressure Error
W(0,1)	9.39E-03	2.75E-01
W(0,2)	9.64E-03	2.04E+00
W(0,i)	1.57E-02	5.64E+00
W(1,1)	9.68E-02	5.12E+00
W(1,2)	9.30E-02	7.41E+00
W(1,i)	1.33E-01	2.32E+01

Mesh Division = 1

Norm	Velocity Error	Pressure Error	Velocity Order	Pressure Order
W(0,1)	2.28E-03	7.20E-02	2.0438171437	1.931573186
W(0,2)	2.27E-03	6.61E-01	2.0838424764	1.623284705
W(0,i)	3.95E-03	2.91E+00	1.986906599	0.9546798578
W(1,1)	4.69E-02	2.41E+00	1.0461466543	1.084555048
W(1,2)	4.59E-02	4.92E+00	1.0185052155	0.5893863754
W(1,i)	6.67E-02	2.28E+01	0.9968686931	0.0232734098

Mesh Division = 2

Norm	Velocity Error	Pressure Error	Velocity Order	Pressure Order
W(0,1)	5.59E-04	2.07E-02	2.0255402807	1.7977589215
W(0,2)	5.79E-04	2.22E-01	1.9745517044	1.5715216098
W(0,i)	9.89E-04	1.50E+00	1.9967001573	0.9593812336
W(1,1)	2.30E-02	1.16E+00	1.0268676669	1.0517406694
W(1,2)	2.28E-02	3.37E+00	1.0089559053	0.5452742667
W(1,i)	3.34E-02	2.26E+01	1.0000001189	0.0102638149

Again the results suggests second order of convergence in space for Velocity and Pressure. Hence we can imply that the Spatial errors dominate over the temporal errors as we used second order interpolation for Velocity and Pressure.

Time convergence – First Order Adams Bashforth method for the time derivative term

By varying the time step around the critical time step (tc) .

For Linear Solution

ux = 2x + y + 3z
uy = - x - 3y - 4z
uz = 6x + 7y - z
p = -5x + 6y + 2z => p(1,1,1)=3, p(0,0,0)=0

For timestep = 2 tc

Norm	Velocity Error	Pressure Error
W(0,1)	1.50E-04	2.40E-01
W(0,2)	1.70E-04	1.38E-01
W(0,i)	2.31E-04	2.08E-01
W(1,1)	9.45E-04	1.46E-01
W(1,2)	1.41E-03	2.46E-01
W(1,i)	4.50E-03	8.46E-01

For timestep = tc

Norm	Velocity Error	Pressure Error	Velocity Order	Pressure Order
W(0,1)	8.08E-05	1.94E-01	0.8968169971	0.3075755411
W(0,2)	9.32E-05	1.10E-01	0.8655542481	0.3296710755
W(0,i)	1.59E-04	1.64E-01	0.5431421649	0.3393416153
W(1,1)	6.00E-04	1.20E-01	0.6556466872	0.2803622943
W(1,2)	9.13E-04	2.11E-01	0.624974104	0.2170540613
W(1,i)	3.20E-03	8.08E-01	0.4906676347	0.0666232624

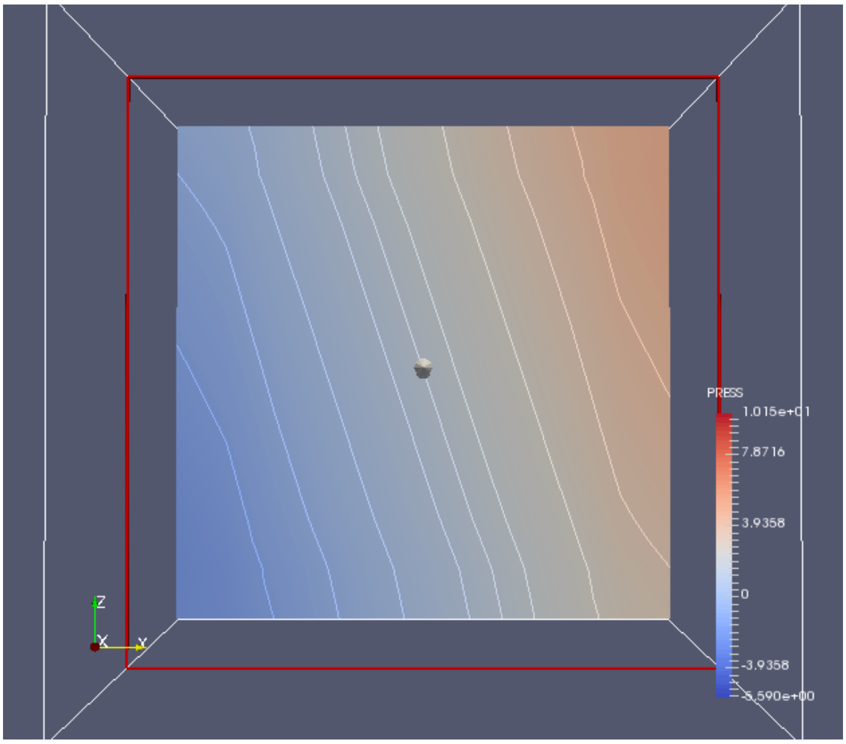
For timestep = 0.5 tc

Norm	Velocity Error	Pressure Error	Velocity Order	Pressure Order
W(0,1)	4.29E-05	1.60E-01	0.9139946715	0.2810565455
W(0,2)	5.10E-05	8.92E-02	0.8691788368	0.2957796233
W(0,i)	1.03E-04	1.31E-01	0.6290938336	0.3221383916
W(1,1)	3.78E-04	1.06E-01	0.6674467691	0.1827979481
W(1,2)	5.89E-04	1.83E-01	0.6330503532	0.2092255646
W(1,i)	2.15E-03	7.65E-01	0.5761186873	0.0791540488

The results suggest first order temporal accuracy for velocity, but poor convergence for pressure.

The poor pressure convergence is theoretically because of the artificial neumann boundary condition for pressure. $\nabla p^{k+1}.n = 0$

However when plotting the pressure contour lines this above condition on pressure contour lines being perpendicular to the surface at the boundaries is not seen.



Second order Adam Bashforth method for taylor green vortex

For time step = 0.25 tc

Norm	Velocity Error	Pressure Error
W(0,1)	9.22E-03	7.93E-01
W(0,2)	9.44E-03	4.55E+00
W(0,i)	1.55E-02	1.39E+01
W(1,1)	9.80E-02	1.91E+01
W(1,2)	9.46E-02	2.16E+01
W(1,i)	1.43E-01	7.26E+01

For time step = 4 tc

Norm	Velocity Error	Pressure Error
W(0,1)	9.80E-03	1.71E-01
W(0,2)	1.02E-02	1.20E+00
W(0,i)	1.58E-02	2.67E+00
W(1,1)	9.58E-02	1.93E+00
W(1,2)	9.20E-02	2.88E+00
W(1,i)	1.23E-01	7.56E+00

There is not much difference in the Velocity and Pressure errors suggesting that the spacial errors dominate the temporal errors. The temporal errors need to be isolated to find the exact temporal order of convergence. To find the temporal errors accurately, it is required to find a solution in the finite element space so that the spacial errors are 0. This has been left as future work.

Using the Rotational form of non-incremental Fractional step pressure correction method

For the linear solution

Errors for the standard form of Fractional step

Norm	Velocity Error	Pressure Error
W(0,1)	2.19E-04	1.44E-01
W(0,2)	2.75E-04	8.08E-02
W(0,i)	6.26E-04	1.16E-01
W(1,1)	2.62E-03	1.01E-01
W(1,2)	3.83E-03	1.60E-01
W(1,i)	1.32E-02	7.45E-01

Errors for the Rotational form of Fractional step

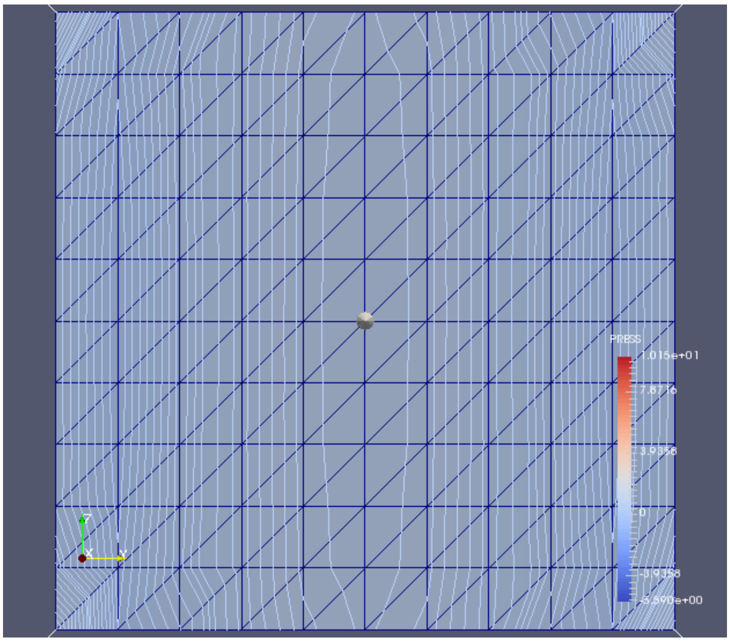
Norm	Velocity Error	Pressure Error
W(0,1)	2.19E-04	3.91E-02
W(0,2)	2.75E-04	2.73E-02
W(0,i)	6.26E-04	9.63E-02
W(1,1)	2.62E-03	1.01E-01
W(1,2)	3.83E-03	1.58E-01
W(1,i)	1.32E-02	7.45E-01

The results suggest that the Rotational form has lead to the reduction in the global error for Pressure. This is an improvement comparing it to the standard form of Fractional step pressure correction method. However, analyzing the pressure contour lines for different cases suggests that the artificial boundary condition, which was theoretically predicted for Standard form of Fractional step methods is not seen when implemented in Alya.

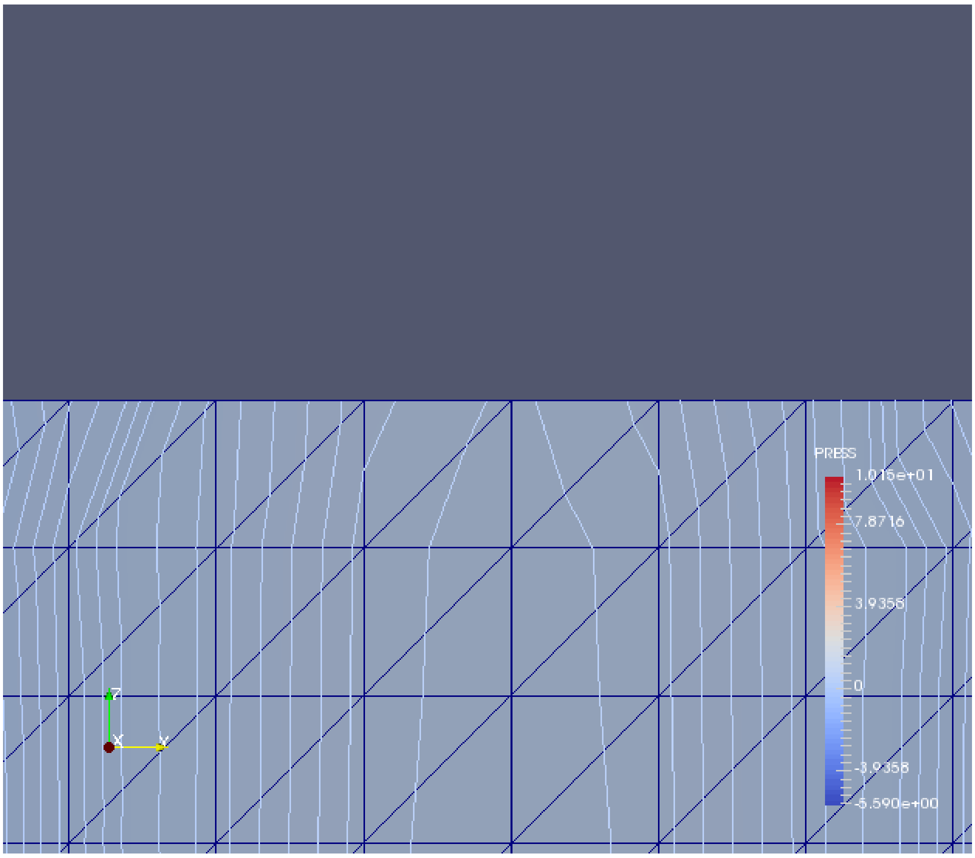
Pressure Contour lines for different cases for Standard FS

1. cubic cavity

for the taylor green vortex



zoomed in

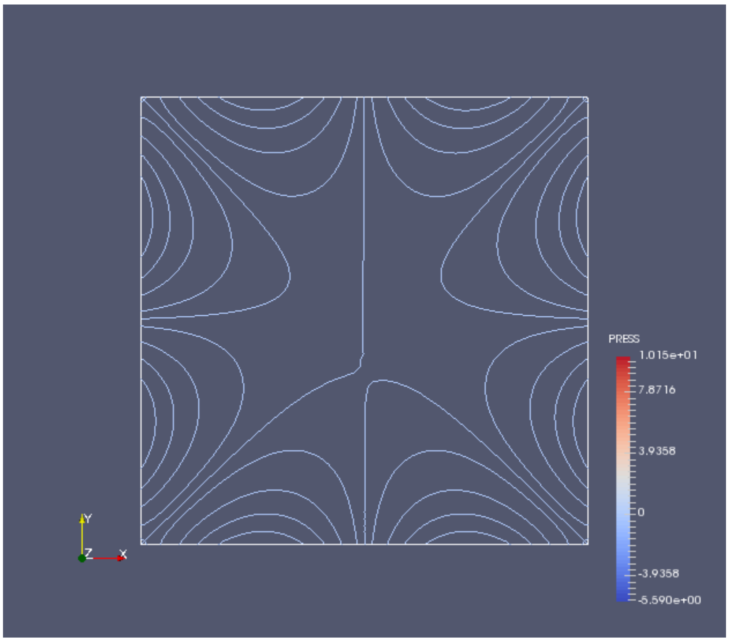


The pressure contour lines are not perpendicular to the surface as was theoretically predicted.

For the 2d cavity

Exact solution from the Guermond paper

$$\mathsf{u}(x, y, t) = \pi \sin t(\sin 2\pi y \sin^2 \pi x, -\sin 2\pi x \sin^2 \pi y),$$
$$\mathsf{p}(x, y, t) = \sin t \cos \pi x \sin \pi y.$$



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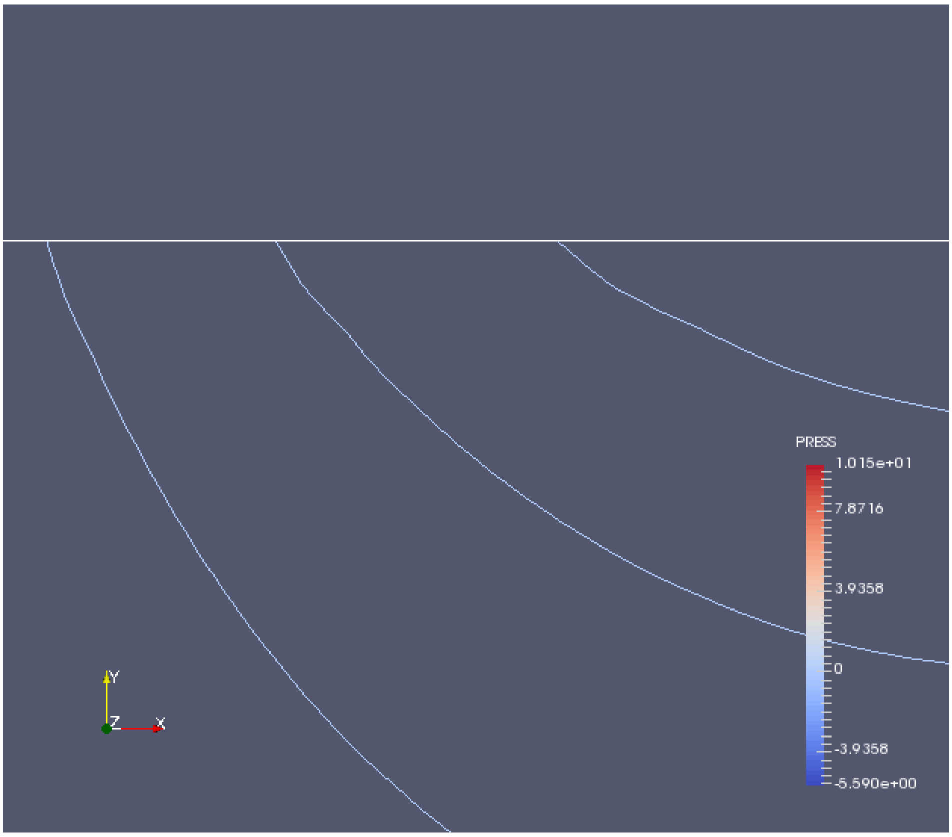
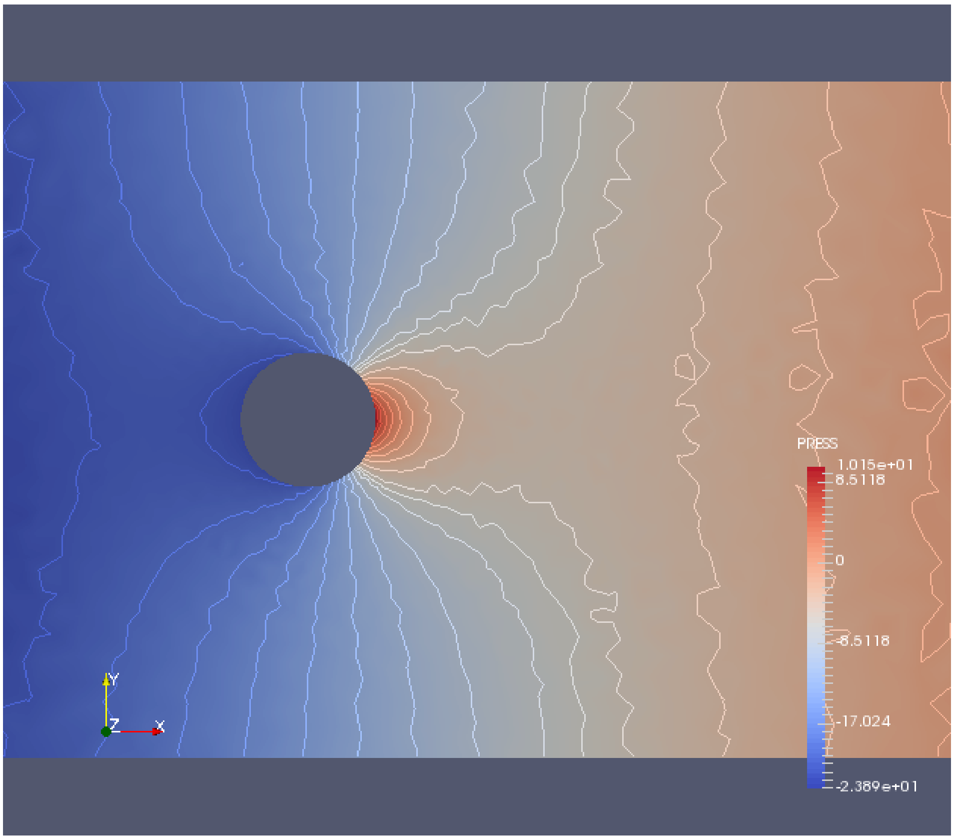
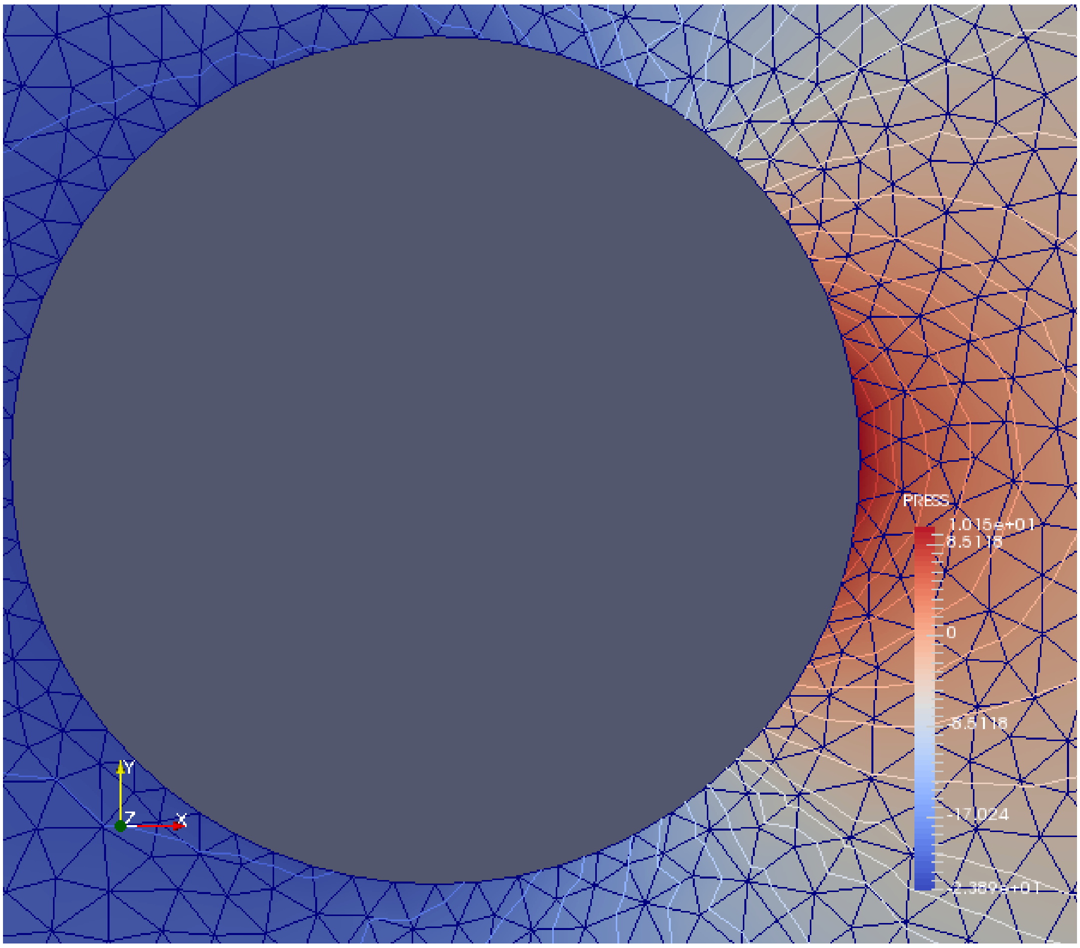


Pressure contour lines are not perpendicular to the surface as was theoretically predicted.

For flow around a cylinder



zoomed in view



Conclusion

- The review of the different fractional step methods – Pressure correction, Velocity Correction, Consistent splitting and Inexact Factorization methods from the Literature was done.

- The Pressure correction method in the Standard and Rotational form was implemented in Alya, a computational mechanics software developed at BSC.

- The implemented code was verified using the method of manufactured solutions. Mesh convergence analysis suggested second order of spacial convergence in Velocity and Pressure as predicted. The special errors dominate the temporal errors, hence the temporal order of convergence could not be found correctly.

- Various cases – Flow in a cubical cavity, Flow in a square cavity, Flow around a cylinder were run in Alya. Even though, the Rotational form of pressure correction method reduced the Pressure error compared to the Standard form, it is found that implementation of the Standard form did not give artificial boundary conditions in the results as was theoretically predicted. Hence, the Rotational form is not necessitated. How the implementation of the Standard form was able to overcome the theoretical problem has to be further investigated.

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