Chair of Scientific Computing
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Time stepping review of open-source solvers

Guided research

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Abstract — The accurate numerical simulation of physical phenomena is crucial in various scientific and engineering disciplines, and open-source solvers offer flexibility and accessibility to researchers and practitioners. A vital aspect of these solvers is the order of the time stepping scheme employed to evolve the solution over time, as it significantly affects the error of the obtained solutions. This project investigates and verifies the order of different time stepping methods implemented on various solvers. We focused on higher-order methods, which give better accuracy and help reduce the computational costs of obtaining a precise enough solution. To study the order of fluid-structure interaction (FSI) simulations using preCICE, we chose OpenFOAM and CalculiX as the studied solvers, which are compatible with this coupling library.
We verified the expected error convergence of second-order methods on both solvers using single-solver simulations and confirmed the correct convergence of first-order methods on FSI simulations. Moreover, we tested higher-order time stepping schemes on FSI simulations and found an incoherent behaviour of the error. We followed by ruling out possible causes of this poor convergence and proposing possible solutions, making this work valuable for future projects aiming to obtain accurate FSI simulations in the preCICE environment.

1 Introduction

- Introduction to coupling simulations (FSI) and to the preCICE library.
- Some brief motivation of performing a convergence study on the known solvers.
- Talk somehow about higer timestepping schemes, and why/when is good to use them. Should you use a higher order timestepping scheme if it doesn't give good results? (No bc it is slower)
- Say we chose this two open source solvers because they are well known and well documented.
- Explain that there is a new version of preCICE which we will also test.
- All the code accessible at repo: https://github.com/atmarc/guided_research/.

2 OpenFOAM

OpenFOAM is an open-source computational fluid dynamics (CFD) software package widely used for simulating and analyzing complex fluid flow problems. Its solver modules employ finite volume methods to numerically solve the Navier-Stokes equations, making it a versatile tool for simulating fluid dynamics in various engineering and scientific applications. In this section we will explain the convergence analysis performed to verify that it has a higher order convergence in time.

2.1 Time stepping schemes

This solver offers various time stepping schemes, and we focused in two for our analysis. The first one is the Euler implicit scheme, as is usually the default one. Given the following partial differential equation:

$$\frac{\partial u}{\partial t} = F(u, t) \tag{1}$$

The Euler implicit scheme would discretize it as follows:

$$\frac{u^{n+1} - u^n}{\Delta t} = F(u^{n+1}, t^{n+1}) \tag{2}$$

This is a first order method, that is quite stable, reason why it is usually the default choice. For the purpouse of this study, we also chose a second order scheme, this being the Crank Nikolson method [1]. This scheme is a combination of an explicit and an implicit Euler step, leading to a second order convergence in time. This method would discretize the previous PDE as:

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{2}\left[F(u^n, t^n) + F(u^{n+1}, t^{n+1})\right] \tag{3}$$

OpenFOAM uses a sligtly different version of this method, by introducing a blending coefficient θ between the Euler implicit method and the Crank Nikolson method. If $\theta = 0$ then we obtain the implicit Euler method, and if $\theta = 1$ then it's Crank Nikolson. For stability, the value $\theta = 0.9$ is recomended in their documentation.

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{\theta}{2}F(u^n, t^n) + \left(1 - \frac{\theta}{2}\right)F(u^{n+1}, t^{n+1}) \tag{4}$$

2.2 Solver parameters

- Talk about the important parameters in the configuration, to obtain accurately enough results, as those where quite time consuming to find. For example, foamToVTK is not accurate enough, and was misleading at the beginning. Also mention the solver used.

2.3 Convergence study

To study the convergence behaviour of OpenFOAM, we focused on the Taylor-Green vortex [2, 3], a standard setup in CFD to validate fluid flow solvers, given that an analytical solution of the case is known. In a 2D, this solution can be obtained by the formulas:

$$u(x, y, t) = -\cos(x)\sin(y)e^{-2\nu t} \tag{5}$$

$$v(x, y, t) = \sin(x)\cos(y)e^{-2\nu t} \tag{6}$$

$$p(x, y, t) = -\frac{1}{4}\left[\cos(2x) + \sin(2y)\right]e^{-2\nu t} \tag{7}$$

where u and v are the horizontal and vertical velocities respectively, p is the pressure and ν is the viscosity of the fluid. This solution holds for a square domain of size 2π. In Figure 1 we can see an example of the computed initial velocities.

We implemented a program that computes the initial velocity for this setup, and writes it into the OpenFOAM configuration. We also wrote a script to automatize the configuration and execution of different setups with varying parameters, so we can perform several experiments automatically. To observe the behaviour of the error, we did several executions of our setup case, fixing all the parameters (grid size, initial velocity, solver tolerances etc.) and changing the time-step size. On our analysis, we mainly focused on the velocity profile.

In a simulation, there are several elements that contribute to the error ε_u. In this study, we were only interested in the error contribution of the time discretization scheme $\varepsilon_{\Delta t}$ to verify the order of the scheme. We assume that the error is formed by $\varepsilon_u = \varepsilon_{\Delta t} + \varepsilon_{\Delta x} + \varepsilon_{\text{num}}$, where $\varepsilon_{\Delta x}$ is the spatial discretization error, and ε_{num} is the error introduced by numerical errors, and other factors. We know that $\varepsilon_{\Delta x}$ is related to the grid size, so we can assume that is constant among the experiments with the same grid size.

There are several possible approaches to study the error. Our strategy was to choose a position cell (i, j) and compare the values of the cell in this position for the different samples. We define as the reference sample $\tilde{u}$, obtained by running the simulation with a $\Delta t = 10^{-5}$. We computed the absolute difference between every sample and the chosen reference solution $|u - \tilde{u}|$ and we plotted them in Figure 2a, for three different grid sizes. As we assumed that $\varepsilon_{\Delta x}$ is constant among the samples with the same grid size, in this plot we obtain

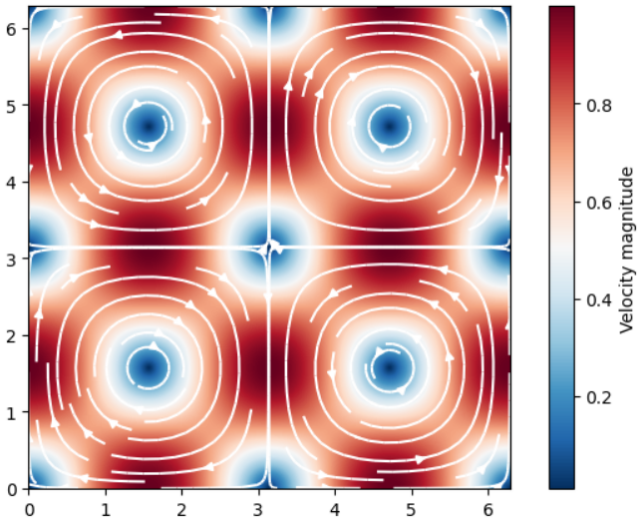
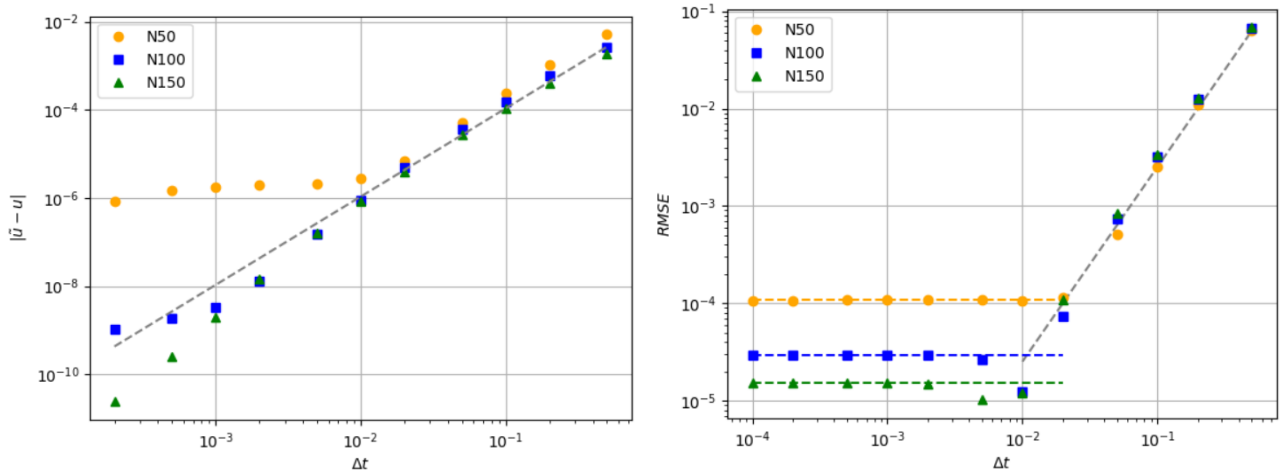


Figure 1



(a) **(b)**

Figure 2 TODO: Caption for both figures

$\varepsilon_{\Delta t} + \varepsilon_{\text{num}}$, allowing us to extract conclusions form the convergence behaviour of $\varepsilon_{\Delta t}$. We can observe how the error decreases when the timestep gets smaller, proportionally to $O(\Delta t^2)$, until a point where the error flattens. Our assumption is that this happens when $\varepsilon_{\Delta t} < \varepsilon_{\text{num}}$, and after a certain point this ε_{num} dominates the entire error. It is also remarkable to see how this point of flattening happens on smaller timesteps for increasing resolutions of the domain.

As me mentioned before, the Taylor–Green vortex scenario has an analytical solution u^*, what allows us to obtain the exact error ε_u of the solutions we obtained, as those are going to be of the form $u = u^* + \varepsilon_u$. To compute this error ε_u, we compute the root-mean-square error (RMSE) of the the velocity flow field, compared to the analytical solution as follows:

$$\text{RMSE} = \sqrt{\sum_{(i,j)} (u^*_{ij} - u_{ij})^2} \tag{8}$$

This is being plotted in Figure 2b, where once again we can observe the error decreasing proportionally to $O(\Delta t^2)$, showing once again a second order convergence in time. In this Figure is very visible the flattening of the error, and how it happens in different points for different resolutions of the domain. This is given that, in this case, the flattening occurs when $\varepsilon_{\Delta t} < \varepsilon_{\Delta x}$, as this time the spatial error is included. This plot also clearly

shows how this spatial error decreases for higher domain resolutions, and gives a clear idea of the magnitude of this $\varepsilon_{\Delta x}$ in these scenarios.

3 CalculiX

CalculiX is an open-source finite element software suite primarily used for solving structural analysis problems. It is designed to simulate the behavior of mechanical and structural systems subjected to various loading conditions. CalculiX provides capabilities for linear and nonlinear static, dynamic, and thermal analyses. It supports a variety of element types, boundary conditions, and material models, making it suitable for a wide range of engineering simulations. In this section, we will overview the timestepping scheme implemented in the solver, and present the convergence study we performed, that displays a higher order convergence.

3.1 Time stepping scheme

The only time-stepping scheme implemented in CalculiX is the α-method [4]. The solver allows the user to select between an implicit or an explicit version of it, and allows to control the α parameter. Moreover, one can define a fixed timestep size, using the DIRECT clause. To get an idea of how this method works, we can start with a given material point with displacement $\boldsymbol{u}$, velocity $\boldsymbol{v}$ and acceleration $\boldsymbol{a}$. We know that the acceleration and velocity are related as such $\boldsymbol{a} = \dot{\boldsymbol{v}}$, and this yields to the following formula to obtain the next timestep values:

$$\boldsymbol{v}^{n+1} = \boldsymbol{v}^n + \int_{t^n}^{t^{n+1}} \boldsymbol{a}(\boldsymbol{\xi}) \mathrm{d}\xi \tag{9}$$

The integral on the right-hand side can be aproximated by a linear combination of $\boldsymbol{a}^n$ and $\boldsymbol{a}^{n+1}$:

$$\boldsymbol{a}(\xi) \approx (1-\gamma)\boldsymbol{a}^n + \gamma \boldsymbol{a}^{n+1} \tag{10}$$

$$\boldsymbol{v}^{n+1} = \boldsymbol{v}^n + \Delta t \left[(1-\gamma)\boldsymbol{a}^n + \gamma \boldsymbol{a}^{n+1}\right] \tag{11}$$

A similar reasoning can be applied to $\boldsymbol{u}$, as $\dot{\boldsymbol{u}} = \boldsymbol{v}$, hence:

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^n + \int_{t^n}^{t^{n+1}} \boldsymbol{v}(\boldsymbol{\eta}) \mathrm{d}\eta = \boldsymbol{u}^n + \Delta t \boldsymbol{v}^n + \int_{t^n}^{t^{n+1}} \int_{t^n}^{\eta} \boldsymbol{a}(\boldsymbol{\xi}) \mathrm{d}\xi \mathrm{d}\eta \tag{12}$$

Assuming again that we can approximate $\boldsymbol{a}$ by a linear convination of $\boldsymbol{a}^n$ and $\boldsymbol{a}^{n+1}$ in the interval $\left[t^n, t^{n+1}\right]$, we can compute the new displacement $\boldsymbol{u}^{n+1}$ as:

$$\boldsymbol{a}(\xi) \approx (1-2\beta)\boldsymbol{a}^n + 2\beta \boldsymbol{a}^{n+1} \tag{13}$$

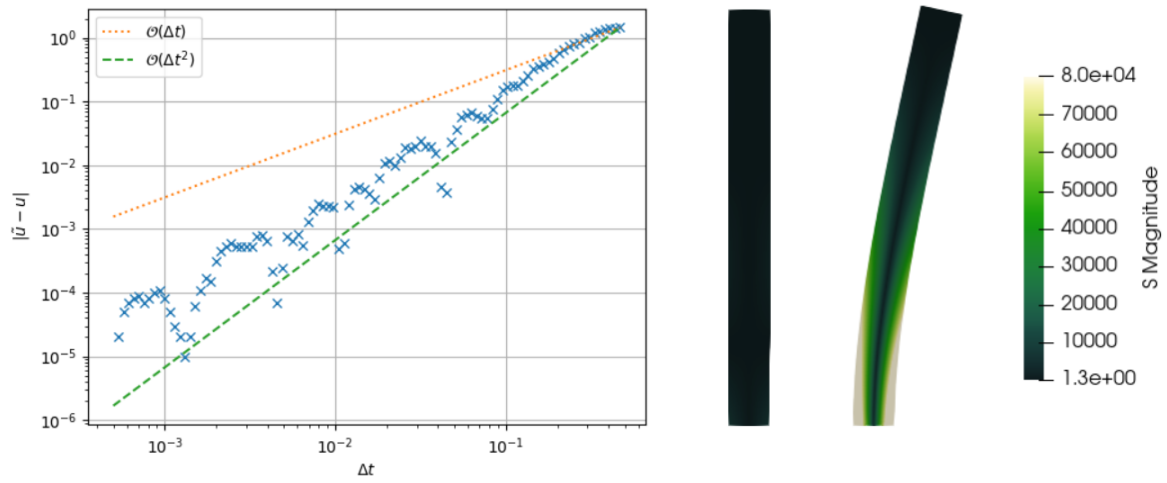
$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^n + \Delta t \boldsymbol{v}^n + \frac{1}{2}(\Delta t)^2 \left[(1-2\beta)\boldsymbol{a}^n + 2\beta \boldsymbol{a}^{n+1}\right] \tag{14}$$

Notice how the linear combinations can be different, so $2\beta \neq \gamma$. This is the basic setup of the α-method, which is proven to be second-order accurate and unconditionally stable for $\alpha \in [-1/3, 0]$, if γ and β satisy that [5]:

$$\beta = \frac{1}{4}(1-\alpha)^2 \tag{15}$$

$$\gamma = \frac{1}{2} - \alpha \tag{16}$$

This α parameter controls the high frequency dissipation, and in CalculiX the value set by default is $\alpha = -0.05$.



(a) TODO: .

(b)

Figure 3 On figure b) we have an example simulation of the elastic flap, showcasing it's elasticity and the displacement of the tip. The colorscale represents the stress of the material.

3.2 Convergence study

In this case, we simulated a solid elastic flap fixed to the floor. A constant force is applied perpendicular to the flap, which is initially resting, which makes it oscillate due to its elasticity. This scenario can be seen in further detail in the solid part of the preCICE perpendicular-flap tutorial [6] or in the code repository of this project.

Given the oscillatory behaviour of the flap, we measured the displacement of the flap's tip over time and used this value for the convergence study. As before, we implemented a script to automatize the execution of the simulations and the post-processing of the output data. We defined a reference solution $\tilde{u}$ as with the OpenFOAM study, which is the one obtained with a $\Delta t = 5 \times 10^{-4}$. The output data format of CalculiX only has 6 significant digits, even though the solver works with double precision values. This means that we could obtain an output with better precision by modifying the solver's routines to export the data, but that rests out of the scope of this work. To circumvent this issue, we defined the simulation parameters so the error was significant enough to be visible in this precision range. This translates to a constant 10N force is applied in the X axis direction, and we take the measurements at $t = 2s$. Then, we plotted the absolute difference to the reference solution $|u - \tilde{u}|$ to observe how the error behaves relative to this solution. One can see in Figure 3 how the error decreases faster than $O(\Delta t)$. With the obtained results, one can definetly argue that the error follows a higher-order convergence, which in certain regions closely follows a second-order convergence. It is also noticeable how for smaller timesteps, the error gets more oscilatory, something that can happen due to the accumulation of other sources of error over time.

4 Coupling the two solvers

We have observed on the previous sections how a higher order convergence is achievable with the OpenFOAM and CalculiX solvers. In this section, we will test them in a coupled simulation making use of the preCICE coupling library. To do so, we make use of the perpendicular flap setup that can be found on the example tutorials of the library [6]. It consists of two components, a two-dimensional fluid flowing through a channel, and a solid, elastic flap fixed to the floor of this channel. The fluid and solid parts of the simulation are computed by OpenFOAM and CalculiX respectively, comunicating between them with the help of preCICE. An example of this setup can be seen in Figure 4.

The flap oscillates due to the fluid pressure building up on its surface during a limited period, given by its initial resting position. The oscillations dampen until the entire system reaches a steady state. We will quantify the error of the simulation by measuring the displacement of the tip of the flap at time $t = 1s$, which is still

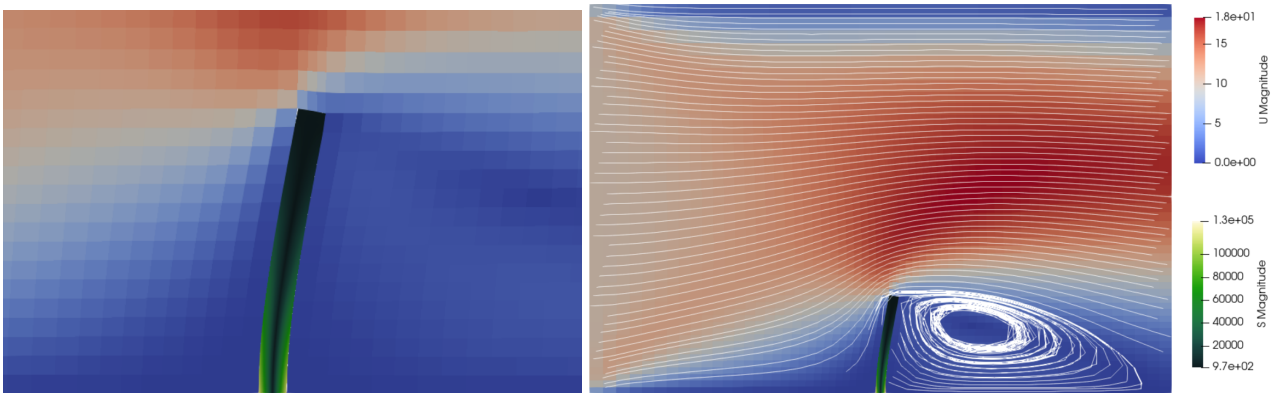


Figure 4 Example solution of the FSI simulation. The left image shows the zoomed in flap, where the stress of the material can be seen in a green scale. On the right image, we observe the whole domain, where we see the magnitude of the velocity field.

in oscilatory behaviour. We wrote specific scripts once again to automatize this task, utilizing similar solver parameters than in the previous sections.

We ran multiple simulations setting the same timestep size on both solvers, and on the preCICE configuration. We also used both the Euler and Crank Nikolson schemes, introduced in section 2.1 for the fluid solver, to observe the difference on their error convergence. Moreover, we ran tests with the stable version 2 and the newest version 3 of preCICE, to observe if the update of the library affected the overall error. In Figure 5 we can observe

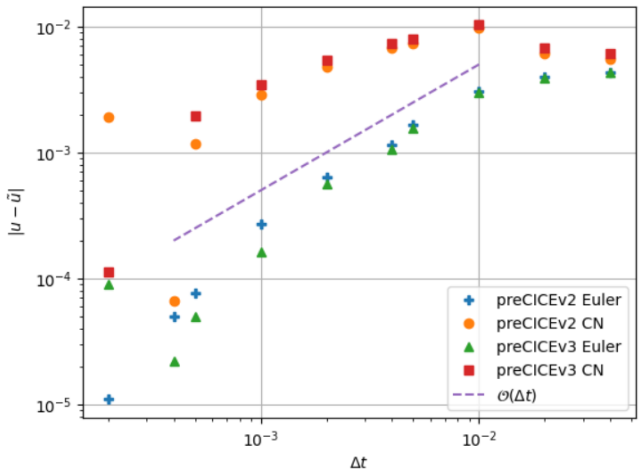


Figure 5 TODO: add title and maybe convergence lines

the results of this experiments. One can observe how using the Euler method, we can achieve a first order convergence of the error. On the other side, we see how the Crank Nikolson method performs poorly in this scenario, giving a worse convergence than the first-order method. It is relevant to mention how the different versions of the code seem to give different results, even though it does not affect the convergence behaviour.

The reasons for the poor convergence of the second-order method can be various. preCICE is a complex environment with many moving many pieces. Each solver has its own adapter, that enables it to be a participant in a partitioned multi-physics simulation. This translates in many possible sources of error. In the next sections we rule out possible sources of error, and propose possible elements that could cause it.

5 Possible sources of error

This section aims to identify and address the potential sources of error we encountered while coupling OpenFOAM and CalculiX using the preCICE library. On section 5.2 we observed that using a second-order

time-stepping method on the fluid solver, gave worse error convergence than using a first-order scheme, despite that both single solver analysis showed higher-order convergences. There are many possible sources of error in this case, starting by the preCICE components. To make sure that the component to blame is not the solid participant, we will test its correct behaviour while coupled to a dummy implementation of the fluid participant. Moreover, we will also test the fluid participant in section 5.2.

5.1 Verification of CalculiX adapter

To interact with a participant solver, preCICE makes use of an adapter, which is an interface between the solver and the preCICE library. To verify the correct behaviour of one of this adapters, one can use a dummy implementation of another participant that only returns some preset magnitudes, and couple both using preCICE.

To test the correct behaviour of the CalculiX adapter [7], we implemented a fake fluid script that could be coupled with CalculiX using preCICE. This fake fluid participant applied a force on the flap with the direction of the positive x axis, substituting what the OpenFOAM solver would produce on the FSI interaction. In this scenario, the returned force by the fake fluid was not constant but varying over time, following $f^n = f_{max} \sin(t^n + \phi)$ on the tip, and decreasing linearly over the height of the flap until reaching a 0 magnitude in the bottom. Our aim was to approximate the forces applied by the fluid on the flap, while making them time dependent to observe a pronounced decrease of the error with a higher-order time stepping scheme.

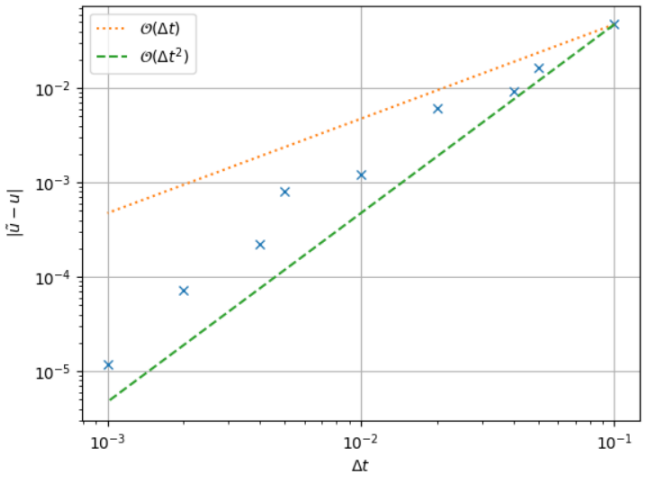


Figure 6 TODO:

In Figure 6 one can observe that the error decreases in a higher-order fashion, as previously observed by the single solver study. This rules out this adapter as the possible source of error, as it showed to give a good error convergence.

5.2 Verification of fluid participant

With the aim of verifying the fluid participant of the FSI simulation, we ran several single-solver simulations, only taking the fluid part of the scenario. The tested case could be seen as a channel with an inverse cavity that stands out, following the geometry of the flap. From this experiments, we observed that this setup was unstable for a high Courant–Friedrichs–Lewy (CFL) number, which is defined as CFL $= \frac{u\Delta t}{\Delta x}$. In the FSI simulation of section , we computed cases with a high CFL number when we had large time-step sizes, which failed to converge in this test. With the aim of improving the stability of the simulation we tried initializing the velocity field with precomputed values of a simulation that reached a steady state.

Once we could obtain some stable simulations, we defined a time-dependent input velocity, so we could observe a decrease of the error when decreasing the time step size. Then, a convergence study of the error was performed, by running the same simulation with the Crank Nikolson scheme, and only varying the time-step size parameter. In Figure **??** we can observe the results of this study, showing how the error does not follow a

higher order convergence. In fact, it's decreasing order is very similar than the one we observed in Figure 5 for the Crank Nikolson scheme. This showcases that the fluid solver was the source of the poor error convergence.

6 Conclusions and future work

- We showed how both solvers can achieve higher order convergence.
- We built a pipeline to automatize running and plotting of solutions, for single and coupled case.
- We made showed how first order convergence is reached in FSI, and how there is no difference between first and second order convergence.
- We showed how for this specific scenario, OpenFOAM and Crank Nikolson do not reach second order convergence.
- We verified the correct behaviour of the Calculix adapter.
- Suggest trying it with other fluid solvers, or trying other scenarios with lower CFL number, but that is still time dependent (transient simulations).

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