Industrial Training

Investigation of Explicit Numerical Time Integration Schemes to solve impact simulations using a HPC framework

Final Internship Report

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Sincerely,

Kiran Kolhe

Contents

1 Introduction:

This is a brief report explaining the study and results of tasks which were carried out at the Barcelona Supercomputing Center during the span of internship. The internship consisted of literature review and investigation of dissipative as well as non-dissipative explicit time integration schemes in order to carry out impact simulations using a High Performance Computing (HPC) framework.

The simulations were performed on MareNostrum IV supercomputer at Barcelona Supercomputing Center using an HPC Finite Element code called "Alya". Alya is a multi-physics simulation code designed to solve coupled problems on supercomputers comfortably. For the purpose, we would be focusing more on the Solid Mechanics module of the HPC code. The module of Alya used to solve Solid Mechanics problems is called "Alya Solidz". Alya uses different solution schemes to solve complex problems. As a matter of fact, in this study the explicit time integration schemes are the center of importance. The Central Difference (CD) scheme which is a non-dissipative explicit scheme and the Tchamwa-Wielgosz (TW) which is a dissipative explicit time integration scheme, both have been investigated with some examples from literature.

2 Review of Explicit Time Integration Solution Schemes:

With the references [1], [3], [5] a literature review of different explicit time integration solution schemes has been performed. Explicit time integration schemes are very robust and straight-forward because of their ease in implementation, but to this advantage we also have to deal with a restriction of these schemes. Explicit methods have a conditional stability, which if not satisfied then the solution becomes unstable. The condition is that the time-step selected for the implementation should be less than or equal to the critical time step to ensure the stability of the problem. Explicit schemes go in the favour of saving the computational costs of problems provided that the time-step size is not very small.
The use of Finite Element Method for space discretization & Finite Difference Method for time discretization gives rise to spurious numerical oscillations. This is because the Finite Element Method lacks the frequencies required to describe wave propagation process properly. This causes the dissipative numerical integration scheme such as TW method, to take part in damping the oscillations.

2.1 Central Difference (CD) Scheme:

The explicit solution scheme such as the Central Difference scheme is used in various software solvers such as Abaqus etc. The Central Difference scheme is the most basic non-dissipative time integration scheme and is used widely because of its ease in implementation. The equations of motion is given by the fundamental formula,

$$M \cdot a = f \tag{1}$$

where M is the mass matrix, a is the acceleration vector and f is the total force vector.
f is given by,

$$f = f^{ext} - f^{int} \tag{2}$$

The internal and external nodal forces are functions of the nodal displacements and the time. The internal nodal forces depend on nodal displacements because of nodal stresses which in turn depend on strains that are calculated from displacements and their derivatives. Whereas, the external nodal forces are prescribed generally as functions of time, but in some cases they may also be functions of nodal displacements depending on structural configurations.

For the Central Difference scheme following are the main equations used for acceleration (a), displacement (d), velocity (v), time (t).

$$a^n = M^{-1} f^n \tag{3}$$

$$\mathrm{v}^{n+1/2} = \mathrm{v}^{n-1/2} + \Delta t^n a^n \tag{4}$$

$$\mathrm{d}^{n+1} = \mathrm{d}^n + \Delta t^{n+1/2} \cdot \mathrm{v}^{n+1/2} \tag{5}$$

Initially, the displacement, velocity, stresses, material state parameters at time zero are initialized to 0. Acceleration at time step 'n' can be found out by evaluating the RHS of (Equ. 3). The RHS can be easily found as the nodal forces at time step 'n' can be deduced form nodal displacements at time step 'n' which are known. Then the velocity can be updated by this acceleration value using (Equ. 4). Note that the velocity is calculated at mid time steps due to central difference scheme. And then finally the displacement at time step 'n+1' can be found by using (Equ. 5).
The time updates used are,

$$t^{n+1} = t^n + \Delta t^{n+1/2} \qquad \textit{and} \qquad t^{n+\frac{1}{2}} = \frac{1}{2}\left(t^n + t^{n+1}\right) \tag{6}$$

The flowchart to implement the steps of this scheme as taken from [1] is as shown below,

Algorithm 1 Flowchart for explicit integration

1: Initial conditions: $\mathbf{v}^0 = 0$, $\boldsymbol{\sigma}^0 = 0$
2: Initialization: $\mathbf{d}^0 = 0$, $n = 0$, $t = 0$
3: Acceleration (assumed as initial value): $\mathbf{a}^0 = 0$
4: Time update: $t^{n+1} = t^n + \Delta t^{n+1/2}$, $t^{n+1/2} = 1/2(t^n + t^{n+1})$
5: 1^{st} partial update nodal velocities: $\mathbf{v}^{n+1/2} = \mathbf{v}^n + (t^{n+1/2} - t^n)\mathbf{a}^n$
6: Update nodal displacements: $\mathbf{d}^{n+1} = \mathbf{d}^n + \Delta t^{n+1/2}\mathbf{v}^{n+1/2}$
7: Enforce displacement boundary conditions. If node I on Γ_D: $\mathbf{d}_I^{n+1} = \bar{\mathbf{d}}$
8: Get forces - assemble rhs $(\mathbf{f}^{n+1} = \mathbf{f}(\mathbf{d}^{n+1}))$
9: Compute $\mathbf{a}^{n+1} = \mathbf{M}^{-1}\mathbf{f}^{n+1}$
10: 2^{nd} partial update nodal velocities: $\mathbf{v}^{n+1} = \mathbf{v}^{n+1/2} + (t^{n+1} - t^{n+1/2})\mathbf{a}^{n+1}$
11: Check energy balance at time step $n + 1$
12: Update counter: $n \leftarrow n + 1$
13: Output; if simulation not complete, go to 4.

Fig. 1: Flowchart for explicit CD scheme. [1]

2.2 Tchamwa-Wielgosz (TW) Scheme:

The literature review of this scheme has been done from [3]. The explicit time integration scheme Tchamwa-Wielgosz (TW), is a dissipative method designed to capture oscillations to a greater extent as compared to the CD scheme. It involves a damping parameter which can be altered to increase or decrease the damping capacity of the scheme. The internal force in TW scheme is lower than the internal force in CD method, which leads to damping of this scheme. The TW scheme with damping parameter equal to 1 will behave exactly the same as CD scheme as it has no numerical dissipation. Variation of different damping parameters depends on different cases and the reader is referred to [3] for more details.

The basic equations for the TW scheme as taken from [3] are,

$$\mathrm{f}^{n+1} = \mathrm{a}^{n+1} + 2\xi\omega \cdot \mathrm{v}^{n+1} + \omega^2 \cdot \mathrm{d}^{n+1} \tag{7}$$

$$\mathrm{v}^{n+1} = \mathrm{v}^{n} + \Delta t \cdot \mathrm{a}^{n} \tag{8}$$

$$\mathrm{d}^{n+1} = \mathrm{d}^{n} + \Delta t \cdot \mathrm{v}^{n} + \varphi \Delta t^2 \cdot \mathrm{a}^{n} \tag{9}$$

Though the TW scheme being first order accurate it damps the overshoots quiet comfortably and quickly. The damping in TW scheme also depends on the size of the time-step. The critical time-step for this method is globally lower, hence this may be a bit expensive method. One important thing about this method is, higher the frequencies are, more dissipative this TW scheme is. The TW scheme smoothes higher frequencies more.

2.3 Critical Time Step:

The critical time-step which is also called as the stable time-step, is an important parameter in explicit time integration. This is a conditional stability which by default comes with explicit schemes. If the time-step of a simulation exceeds the critical value, then the solution grows unboundedly. The stable time-step is given by,

$$\Delta t = \alpha\, \Delta t_{critical} \qquad and \qquad \Delta t_{critical} \leq \min \frac{l_e}{c_e} \tag{10}$$

where l_e is the characteristic length of element e, $c_e$is the current speed of wave in element e, α is a reduction factor that accounts for the destabilizing effects of nonlinearities ($0.8 \leq \alpha \leq 0.98$). The mesh time step is obtained from element time steps. For each element, an element time step is calculated and the minimum element time step of all is chosen as the mesh time step.

Now, having studied some points about these explicit time integration schemes, let us see how they behave when they are used to solve problems. First, the schemes would be validated for a simple cantilever beam test and on obtaining successful results in that, a complex engineering problem would be analysed with those schemes to check the performance.

3 Cantilever Beam Test:

The CD and TW solution schemes described earlier would be used to analyze the effect of load on a cantilever beam. An explicit dynamic analysis of the cantilever beam is made to watch its out-of-plane bending. As regular as it seems, the boundary conditions applied to the cantilever beam are, fully supported at one end, and concentrated one step load is applied at the free end. The dimensions of the beam are 6000 x 200 x 100 mm. A mesh of 6 elements is played initially.

As far as the results are concerned, both the solution schemes are compared for different parameters and the behavior is observed. Also, the results have been compared to a reference solution taken from [7]. Different results such as comparison of the displacement-time curves for the solution schemes are seen, comparison between different mesh refinements for a particular solution scheme have been done, comparative difference in implementation of schemes with sequential computation and parallel computation of processors has been observed, comparison of different time-steps required for the problem etc. all these things have been analyzed in the beam test.

3.1 Results:

In this section, the cantilever beam case has been analyzed in different ways for the comparison of both the solution schemes.

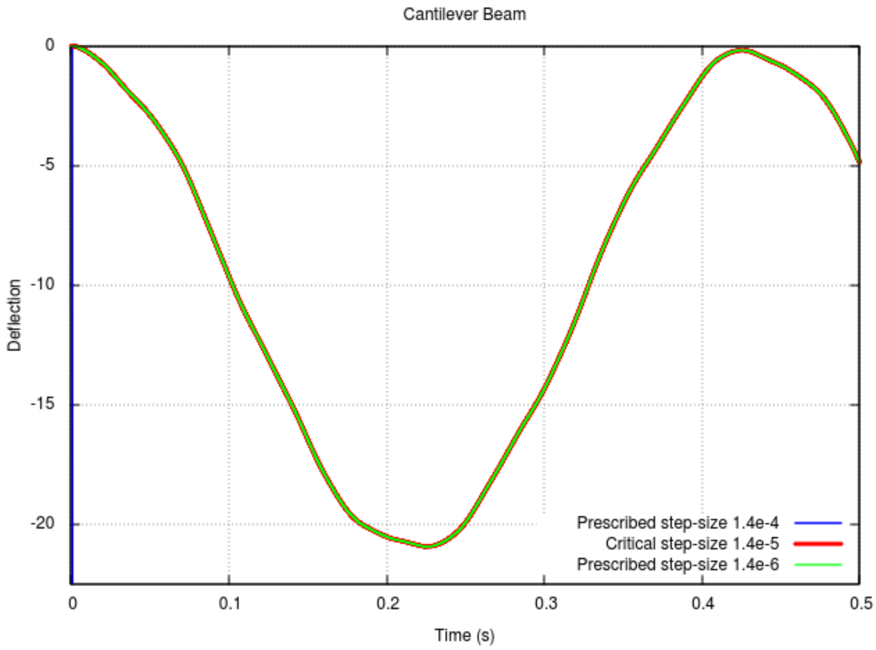

Fig. 2: Comparison of Different Time-step sizes

Fig. 2 shows the plot of different time-step sizes used in computation by the CD scheme. The default critical time-step size is 1.4e-5 s which is taken from the reference solution paper [7]. The critical time-step size can also be verified by running the simulation by using just 1 time-step. The value which it gives is 1.46904e-5 s. The other time-step sizes plotted in the graph are, one whose value is below the critical limit (1.4e-6 s) and the other which is above the critical limit (1.4e-4 s). It is very important to note that, in explicit time integration the step size should always remain less than or equal to the critical time-step size. As observed from the plot, since the time-step size of 1.4e-4 s is greater than the critical limit of the problem, the result is totally unstable represented by the vertical line on Y-axis. The rest 2 time-step sizes yield good results.

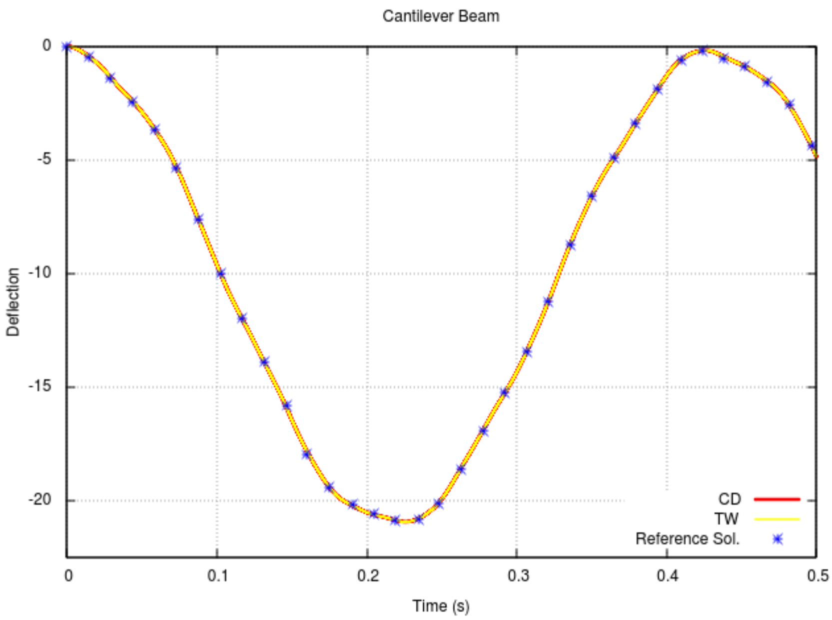

Fig. 3: Comparison of CD and TW solution schemes with reference solution

Fig. 3 shows the displacement-time comparison between the reference solution, CD scheme ad TW scheme. It is observed that both the schemes are in range with the reference solution which concludes that the results obtained are stable.
It is observed that with the default parameters, both the CD and TW schemes achieve total simulation time of 0.5 s in 35715 time steps. The number of processors used for running the simulation were 4.

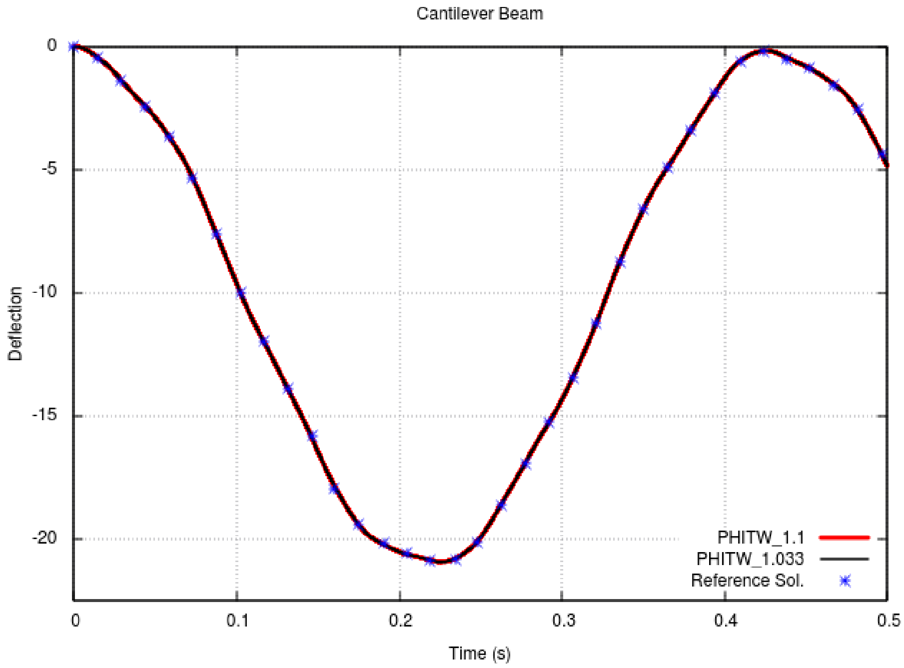

Fig. 4: Plot for different Damping parameter values for the TW scheme

Fig. 4 shows a plot for different values of the damping parameter used in the TW scheme. The damping parameter is symbolized by PHITW.

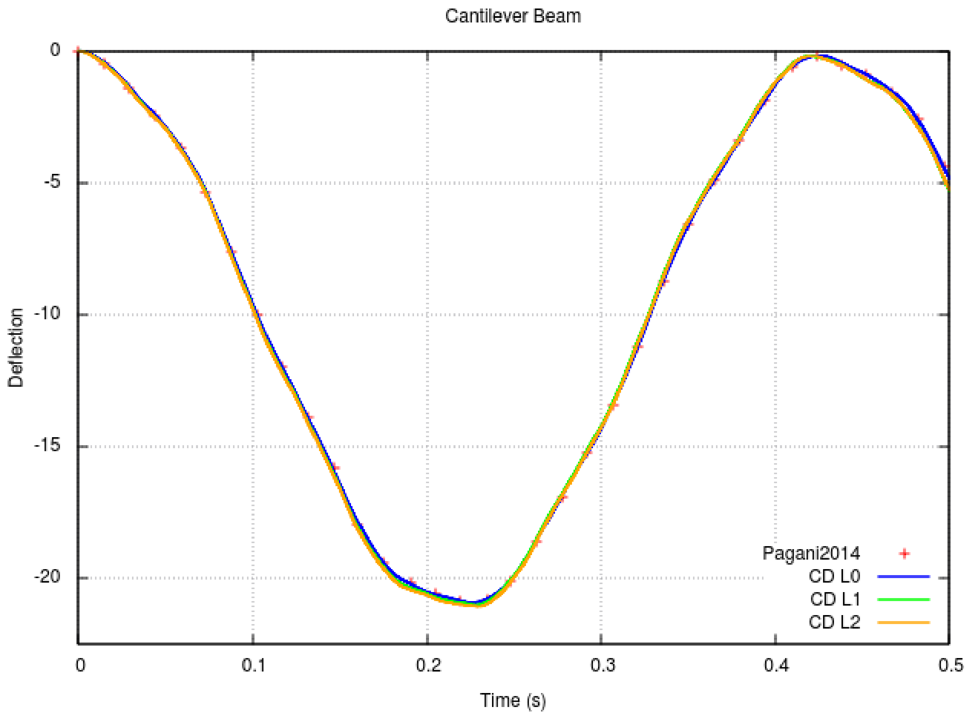

Fig. 5: Comparison of different mesh levels (refinements) for CD scheme

Fig. 5 represents the displacement-time curve for different mesh refinement levels for the CD scheme. The different mesh levels have also been compared with the reference solution indicated by 'Pagani2014' in the plot. In the graph, the L0 mesh level is computed with the time-step size of 1.4e-5 s, while the L1 and L2 mesh levels have been computed with size of 1.4e-6 s. It is very important to note that, as we decrease the element size, i.e refine the mesh, the time-step size also should be reduced or else we get unstable solutions. The behavior can be seen in the curve.

Fig. 6 to **Fig. 8** represent the GiD visualizations for different mesh levels (refinements).

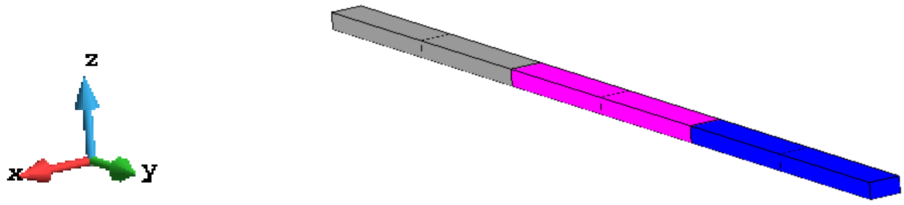

Fig. 6: Visualization for Level 0 mesh

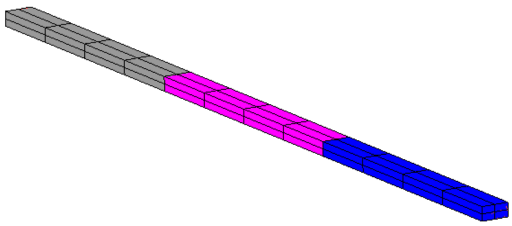

Fig. 7: Visualization for Level 1 mesh

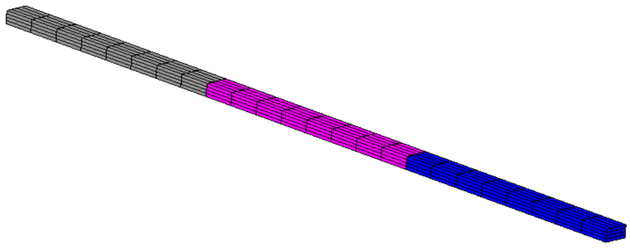

Fig. 8: Visualization for Level 2 mesh

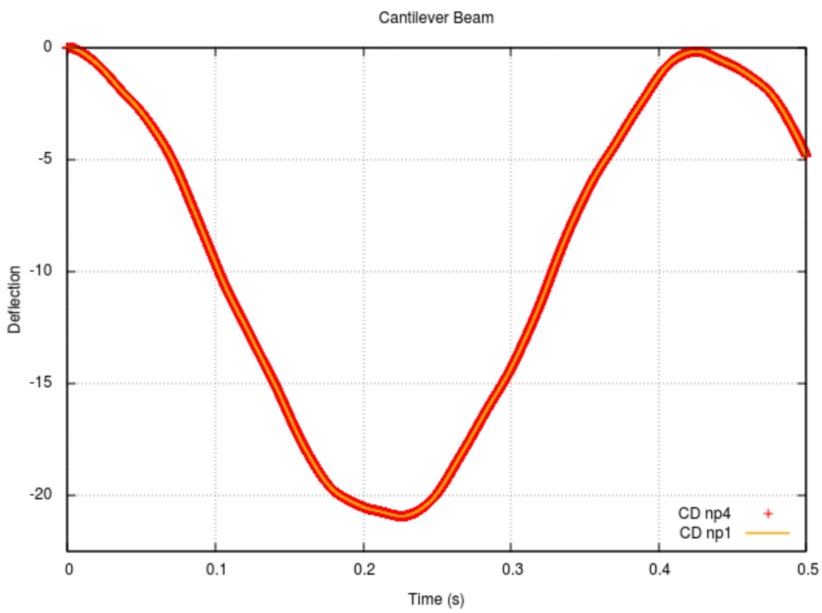

Fig. 9: Comparison for CD scheme using different number of cpu's

To compare if the results are same with sequential computing (i.e using 1 cpu for computation) and parallel computing (i.e using 4 cpu's), the graphs have been plotted in **Fig. 9** for the CD scheme. And as expected, the curves exhibit exactly the same behavior thus proving that the scheme works totally well even if we change the number of processors used.

The load applied on the cantilever beam causes its deflection at the free end which is shown in **Fig. 10**. The results have been visualized in GiD. The maximum displacement can be observed at the right-most end where the load is applied.

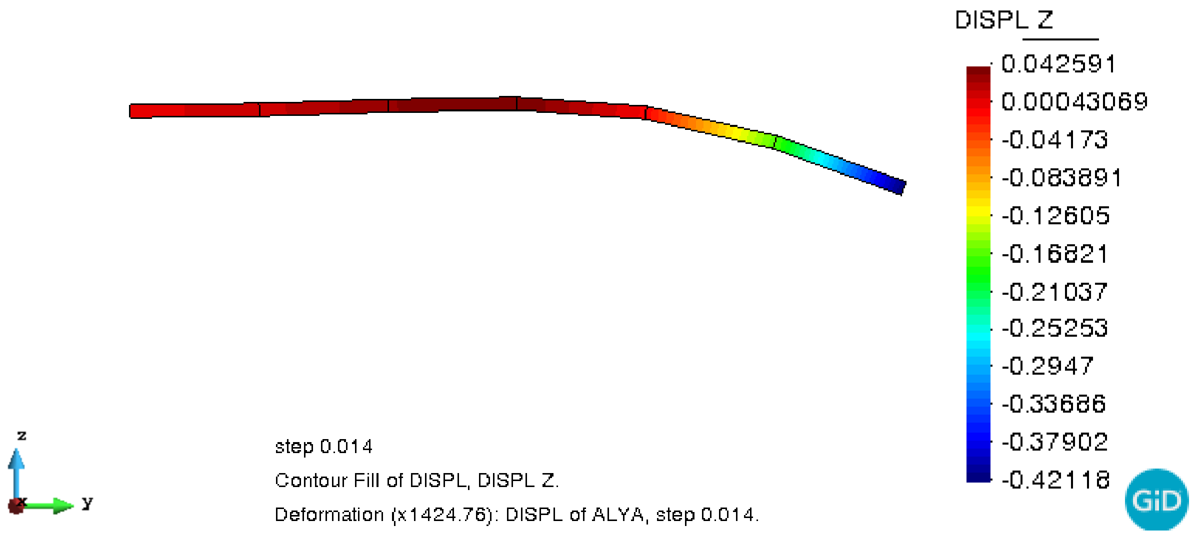

Fig. 10: Deformed cantilever beam

Looking at the results and dynamics shown, we can predict that the solution schemes work well for the implemented case.

4 Low Velocity Impact Test:

Now, the CD & TW solution schemes have been tested for a more complex engineering problem in order to verify its robustness. In this section, a low velocity drop-weight impact test has been performed. This simulation considers the impact of an impactor on a structure which is taken as plate. The impactor which is taken as a rigid body is dropped from certain height above the plate, and its impact on the plate is observed. Now, the height from which the impactor should be dropped is given by a simple basic calculation involving the potential energy because of the height given by,

$$h = \frac{E}{mg} \tag{11}$$

where E is the energy required to perform the impact test, m is the mass of the impactor, g is the gravitational acceleration taken as 9.81 m/s^2. We consider the gravity loads in this simulation test as the weight of impactor is also considered in the parameters. The impactor is specified with an initial velocity before the impact given by,

$$v = \sqrt{\frac{2E}{m}} \tag{12}$$

With the explicit solution schemes used, the Dynamic transient analysis is performed for this impact simulation test. The impact test is performed for an Energy of 10J since it is a low velocity impact test with the impact time of 5 ms and keeping a gap of 0.1 mm between plate and the impactor. The radius of rigid body impactor is 8 mm while its mass is taken as 2 kg. The material used for plate is T800/M21 laminated composite. Also, intra-laminar damage model is used for prediction of fiber/matrix failure and cohesive elements for delamination prediction.

The maximum force by which the impactor hits the plate is somewhere around 5200 kN which can be seen in the force-time curve (**Fig. 17**) shown in the succeeding sections.

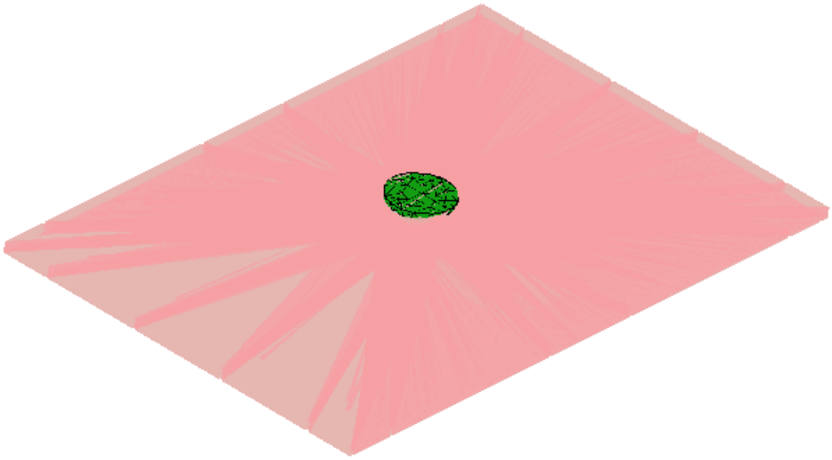

Fig. 11: Impact test set-up showing plate and impactor

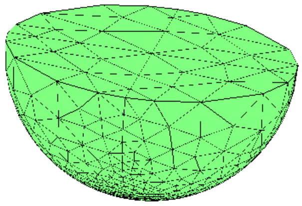

Fig. 12: Impactor Geometry

4.1 Results - Visualizations:

Fig. 13 represents the output files as visualized in GiD for the impactor and the plate. These have been plotted for the TW scheme. As observed, the impact has been done at the center of the plate where maximum displacement has been observed.

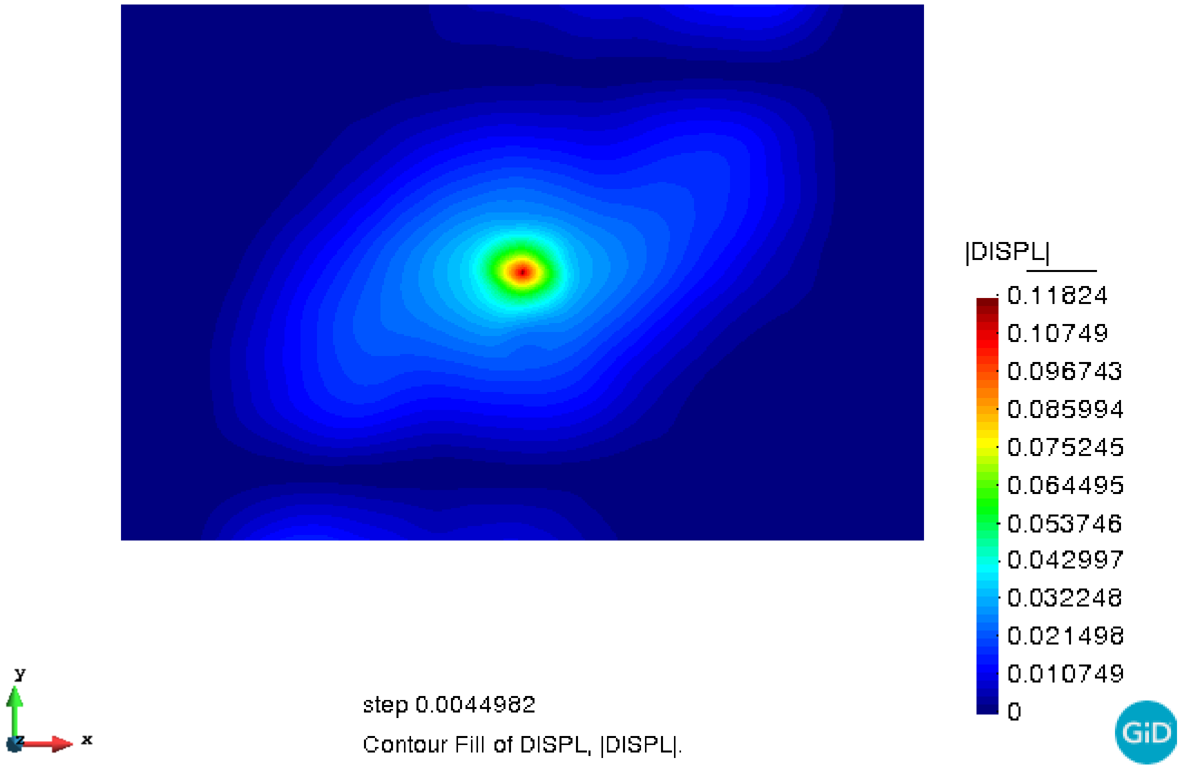

Fig. 13: Contour fill of plate for displacement after the impact

The deformations have been visualized with a deformation factor approximately near to 100 in GiD in **Fig. 15**.

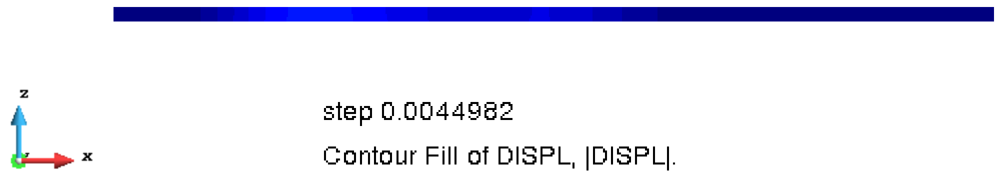

Fig. 14: Undeformed plate before the impact

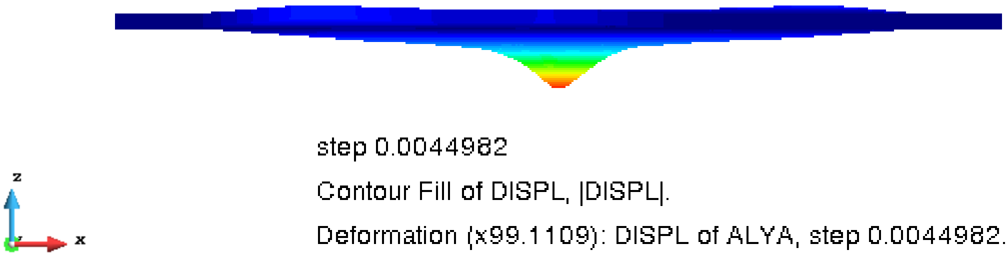

Fig. 15: Deformed plate after impact

4.2 Results – Graphs:

In this section, we compare different plots involving important parameters for the CD and TW solution schemes. For this case, a total of 626 cpu's have been used for the analysis in MareNostrum 4 using Alya FE code. The damping factor for the TW scheme has been set to 1.033.

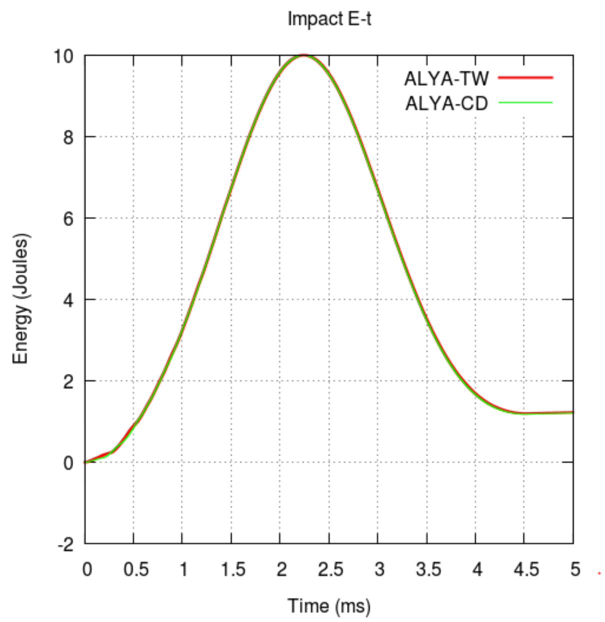

Fig. 16: CD & TW comparison on Energy-Time plot

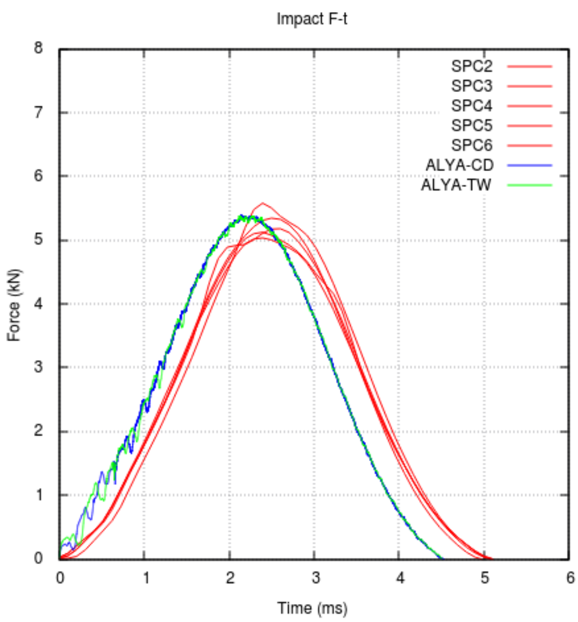

Fig. 17: CD & TW Comparison on Force-Time plot

Fig.16 shows the plot of energy vs time for both the solution schemes. From the plot it can be observed that both the schemes show almost the same behavior in dissipation of energy. Theoretically, the energy by which impact has been performed (which is 10 J) should be returned back after the impact. This means that if the curve starts from zero, it should end back at zero. But, as observed from the plot, it can be noticed that not all energy used for the impact is returned back. This is because of the basic reason that, some of the energy is dissipated in this impact simulation due to damage. Hence, in the graph we can see that there is some difference in the energy level at start and the energy level at end of the impact. This difference is the dissipated energy which is around 1 J.

Fig. 17 shows the comparison of behavior of both the solution schemes for force evolution during the impact with the specimen results obtained from experimentation. It is noted that both the schemes exhibit similar behavior for the force evolution over given time. The maximum possible force reached in the impact is approximately around 5200 kN which can be identified from peak of curve in the graph. The curve increases as the impact takes place. And then we can observe a fall in the curve which is a representation of the impactor returning back to its original position after the contact has happened.

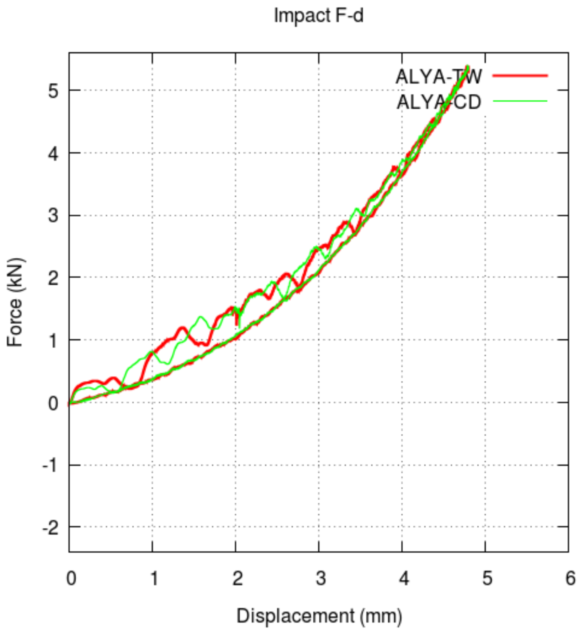

Fig. 18: CD & TW comparison on Force-Disp. plot

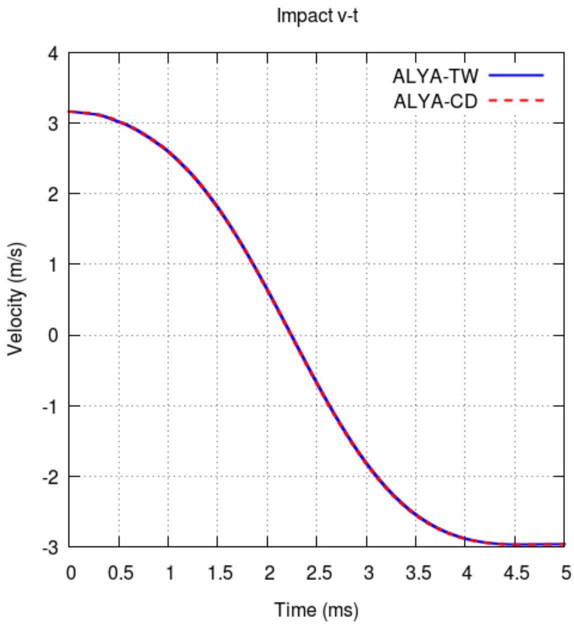

Fig. 19: CD & TW Comparison on Velocity-Time plot

Fig. 18 shows the force vs displacement behavior of the CD and TW schemes. It can be observed that as the force increases the displacement also increases which seems logical.

Fig. 19 represents the evolution of velocity with time for both the solution schemes. As easy to observe, it can be seen that both the schemes make no difference in showing the velocity behavior of the impactor. As mentioned earlier, the impactor is specified with an initial velocity in order for the impact to take place. The initial velocity specified is 3.162 m/s. Hence, the curve starts from initial prescription and not zero, and as the impact comes to an end the velocity also reduces to constant.

5 Conclusions:

1. In this report, a review of some explicit time integration solution schemes such as Central Difference scheme and Tchamwa-Wielgosz scheme was done and these solution schemes were tested for different examples.
2. From the results obtained, it can be verified that the dynamics were well organized and the solution schemes yielded good results for simple case of cantilever beam as well as the complex problem of drop-weight impactor test.
3. It is very important to note that, in the explicit time integration, critical time-step size of the computation plays a very important role. In order to be sure that the analysis should work well with the explicit schemes, it is always necessary that the time-step size given to the solver should never be more than the critical time-step size required for the solution. If it exceeds the critical limit, then the kinematics are not well predicted and the solution becomes unstable.
4. But, one more thing should be taken care of is, the time-step size should not be very small, because the smaller the time-step size is, the more the cost of computation would be. Hence, it is very necessary to find out a suitable time-step size which is also closer to and smaller than or equal to the critical time-step size of the solution. This is in regard to have good results at a suitable computational cost.
5. Numerical dissipation is a tool to be used with precaution as it can lead to a loss of accuracy when dissipation increases. As dissipation increases, number of time steps increases, thus computational time increases and therefore the method becomes more expensive.

6 References:

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