Comparative study of numerical explicit time integration algorithms

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Abstract

The aim of this research is to make a comparative study of numerical explicit time integration algorithms used in the domain of shock and impact. Numerical simulation of such problems, with explicit algorithms for time integration, involves very small time steps for reasons of stability. Thus, very high numerical frequencies can be found in the final solution in displacement or stress. But generally the high frequencies and mode shapes of the spatially discretized equations do not accurately represent the behavior of the original problem. It is proved that algorithms such as Chung-Lee, Zhai, HHT, Tchamwa, central difference method, are useful to solve problems including high speed phenomena. The different regions of stability, accuracy, but also the capacity of each numerical scheme to smooth very high frequencies are compared. Finally, these integration schemes are implemented in the HEREZH++ finite element code developed at the LG2M laboratory ([1]). For some simple problems the solutions obtained from HEREZH++ and the commercial code LS-DYNA are compared and discussed. For instance, following these simulations, it seems that the Tchamwa’s algorithm is particularly efficient to smooth the highest frequencies.

1 Introduction

The dynamic behavior of materials arouses an increasing interest. Our subject is related to the time-dependent mechanics of the deformable solid modelled by finite elements, although the presented methods can apply to fluid mechanics.

The usual method is to carry out two distinct discretizations, one for space and one for time. The space discretization uses the shape (interpolation) functions of
the parametric coordinates of the interconnected finite elements to track the particles through time. The time discretization can use various schemes of resolution; the objective is, of course, to reduce the number of unknown factors to be managed. These methods are classified in two categories, single-step and multi-step schemes. As the bibliography shows that single-step schemes are the best compromise between computation time and data storage, we will focus on them. One can refer to Chung-Lee [5] for an exhaustive presentation. Among single-step scheme, one distinguishes the explicit and implicit methods. Explicit solution techniques have certain advantages. For example, the time increment is only dependent on the element size and material properties as the stiffness matrix is not computed, and CPU cost per time step is proportional to the number of d.o.f. However, this method is conditionally stable, as the time step must be less than a critical one based on the highest eigenvalue of the mesh. The implicit finite element method has the advantage to be unconditionally stable with respect to the time step size. However CPU cost per time step is roughly proportional to the square number of d.o.f. of the model, as the stiffness matrix has to be computed and reversed. Usual algorithms for explicit and implicit method are respectively the central difference method and the Newmark method. One can refer to Geradin [3] for a presentation of these methods, and to Belytschko and Hughes [2] for the study of the stability and the convergence of these algorithms. In the last few years, new techniques appeared ([5] [7] [6]). The theoretical study of their stability, precision and convergence resulted in defining the optimum parameters for their use. But these studies are carried out on a continuous problem whereas their interest lies in their capacity to filter the frequencies induced by the finite element spatial discretization. In this paper, various algorithms are presented and implemented in the HEREZH++ finite element code which is developed in C++.

2 Algorithms

The reader can see Belytschko and Hughes [2] for a presentation of usual algorithms and the well-known HHT method. We can also refer to the works of Chung-Lee [5], Zhai [7] and Tchamwa-Wielgosz [6] for a precise explanation of the new algorithms.

Our study focuses on the Tchamwa-Wielgosz model (noted Tchamwa). The study of stability is done following the same method as presented by Hughes.

The local equilibrium equations are approximated by virtual power principle. Time-stepping scheme uses a constant time step length $\Delta t = h$ for simplicity. We note $n$ or $t$ the time corresponding to $t = n\Delta t$.

Tchamwa method:

$$M\ddot{X}_{n+1} + f(\dot{X}_{n+1}, X_{n+1}) = g(X_{n+1}, t)$$ (1)

$$\dot{X}_{n+1} = \dot{X}_n + \lambda h \ddot{X}_n$$ (2)

$$X_{n+1} = X_n + \alpha h \dot{X}_n + \beta h^2 \ddot{X}_n + \gamma h \dot{X}_{n+1}$$ (3)
Where $\alpha$, $\beta$, $\gamma$, and $\lambda$ are the parameters of the numerical scheme and $X$ the position vector.

As time and spatial discretization are independent, one can use a simple mesh to underline the damping properties of the numerical scheme. Let us consider the simple problem of a single beam element (length=200 mil, section=4 mm$^2$, density=8.10$^{-9}$ kg/mm$^3$) fixed at one end, with an initial velocity (1 m/s) at free end. Figure 1 shows the influence of $\phi = \beta + \gamma$ on the damping of the displacement of the free end (cf.3.1).

![Figure 1: Influence of $\phi$ parameter on the damping of the displacement of the free end of a single clamped beam element.](image)

In this model of one degree of freedom, only one frequency exists which is then the highest one. So the attenuation should be directly seen. But this frequency is also the lowest one, so an high value of $\phi$ is here necessary to obtain an appreciable attenuation.

An accurate mesh, 100 elements, cf. figure (7) leads to a larger frequency band and allows to point out the amount of attenuation on high frequency.

### 3 Implementation

Different algorithms have been implemented in our software Herezh++ developed in C++. Object orientation has been used in order to obtain easy developments. We will now present the different object-concepts used with success in this implementation.
Clamped beam with initial velocity on free edge

Figure 2: Comparison between the different methods

Data encapsulation is here systematically selected, i.e. data IO access are made by methods. Then data modifications can perfectly be controlled in particular with regard to their coherence. This practice improves independence between classes.

Each time integration scheme is implemented into a specific class which inherits a generic one. This virtual top class is used as interface. This concept is fundamental to easily allow the addition of new algorithms without modifying the remainder of the program. Five dynamic algorithms have been implemented in Herezh++: Newmark, Tchamwa-Wielgosz, central difference method, Zsai, Chung-Lee.

The algorithm implementation is greatly simplified by the global handling of certain data types such as all the degrees of freedom to various times: \( t, t + \Delta t, t - \Delta t \). For that, the solution consists in storing these types in global containers like vectors or tables. However these data are defined at nodes and have to be managed in order to keep coherence with the coordinates at various times. Thus it is logical to define a node-object which is in charge of this data management. In this case the principle of encapsulation will be broken by the global container manipulation. A solution is to use two storages for the same data, the first and main one is in object node, the second is intermediary to global containers. In order to optimize data transfer between these two storages, an indirect addressing is set up in the two directions.

In the central difference method although the speed and acceleration appear in the equation, it is possible during the implementation to use only degrees of freedom related to the position at three moments: \( t, t + \Delta t, t - \Delta t \). The fact of
handling only one type of d-o-f facilitates the variable management. However it can’t be accepted in a general framework for coupling problems which necessarily introduce different types of d-o-f.

In particular in the case of the new algorithms: Zsai, Chung-Lee and Tchamwa, it seems preferable to introduce speed and acceleration d-o-f. For that, the concept of d-o-f active or not is introduced for a given variational formulation.

In our case the weak form of the equilibrium equations is used to obtain the field of acceleration. The d-o-f of speed and acceleration are directly obtained by the other vector relations (cf. 2 and 3 for instance).

Various types of matrix storages are implemented for the mass matrix: diagonal, square, band, sparse. In particular it makes it possible to study the importance of the diagonalisation of the consistent mass matrix.

With regard to the implementation the concept of abstract class is naturally used to define a class of abstract matrix which will be used as interface with all algorithms.

In the case of square and band matrix, we can use the fact that mass matrix is constant with time step to optimize linear system resolution. In our case, a direct method of Cholesky is used. The stage of triangulation is carried out at the beginning of calculation, increment 0. At each increment we only need to solve the two linear problems with triangular matrices. On the other hand in the case of storage out of sparse matrix, the implemented iterative methods of combined Bi-gradient type do not allow any preliminary simplification.

Various classical linear and vectorial matrix operations are overloaded. Thus the implementations of the algorithms are independent of the matrix type. However operations between two different types of matrix are not authorized except between diagonal matrices and the other types. Indeed, it does not seem logical to use a sparse matrix for the mass and a band matrix for the stiffness for instance.

3.1 Convergence: consistence and stability for Tchamwa-Wielgosz scheme

Consistency study of Tchamwa algorithm leads to \( \lambda = 1 \) and \( \alpha + \gamma = 1 \). After linearisation of the equation (1), we obtain:

\[
\begin{align*}
M \ddot{X}_{n+1} + C \dot{X}_{n+1} + K X_{n+1} &= F_{n+1} \\
\dot{X}_{n+1} &= \dot{X}_n + h \ddot{X}_n \\
X_{n+1} &= X_n + h \dot{X}_n + h^2 \ddot{X}_n
\end{align*}
\]  

If we consider a Rayleigh damping, the equation of motion in modal coordinates \( \mathbf{q} \) becomes:

\[
\ddot{q}_{n+1} + 2 \xi \omega \dot{q}_{n+1} + \omega^2 q_{n+1} = G_{n+1}
\]

where \( \omega \) is the undamped frequency of vibration, and \( \xi \) is the modal damping ratio.

In matrix form this leads to:

\[
\begin{pmatrix}
\dot{q}_n \\
\ddot{q}_n
\end{pmatrix} + \begin{pmatrix}
2 \xi \omega & \omega^2 \\
\omega^2 & 2 \xi \omega
\end{pmatrix}
\begin{pmatrix}
\dot{q}_{n+1} \\
\ddot{q}_{n+1}
\end{pmatrix} = \begin{pmatrix}
G_n \\
G_{n+1}
\end{pmatrix}
\]

where \( L_n \) is the load vector and the expression of the amplification matrix \( A \) is:
Following the method used by Hughes ([4]), one can show that numerical scheme is stable if the following criteria are fulfilled.

If $\xi = 0$, \[\begin{align*}
2 + \left(\frac{1}{2} - \phi\right) \Omega^2 &\geq 0 \\
2 + (1 - \phi) \Omega^2 &\geq 0 \quad \text{and} \quad \phi = 1 \\
(1 - \phi) \Omega^2 &< 0
\end{align*}\]

If $\xi \neq 0$, we have the following systems

\[\begin{align*}
2 - 2\xi \Omega + \left(\frac{1}{2} - \phi\right) \Omega^2 &\geq 0 \\
2 - 2\xi \Omega + (1 - \phi) \Omega^2 &\geq 0 \\
-2\xi \Omega + (1 - \phi) \Omega^2 &< 0
\end{align*}\]

\[\begin{align*}
(1 - \phi) \Omega - 2\xi &= 0 \\
\Omega &> \frac{-2\xi}{\phi} \\
\Omega &< \frac{-\xi + \sqrt{\xi^2 + 4\phi}}{\phi}
\end{align*}\]

Studies of the different cases can be summarized by next tables.

- For $\xi = 0$

<table>
<thead>
<tr>
<th>Condition on $\phi$</th>
<th>Condition for stability</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi \geq 1$</td>
<td>$\Omega &lt; \sqrt{\frac{2}{\phi - \frac{1}{2}}}$</td>
</tr>
</tbody>
</table>

- For $\xi \neq 0$

<table>
<thead>
<tr>
<th>Conditions on $\phi$</th>
<th>Conditions for $\xi$</th>
<th>Stability</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi = 1 - \frac{2\xi}{\Omega}$</td>
<td>$\forall \xi$</td>
<td>$\Omega &lt; 2$</td>
</tr>
<tr>
<td>$\phi &lt; \frac{1}{2}$</td>
<td>$\xi \leq \sqrt{1-2\phi}$</td>
<td>unconditionally</td>
</tr>
<tr>
<td>$\phi &gt; 1$</td>
<td>$\forall \xi$</td>
<td>$\Omega \leq \frac{-\xi + \sqrt{\xi^2 + 2(\phi - \frac{1}{2})}}{\phi - \frac{1}{2}}$</td>
</tr>
<tr>
<td>$\frac{1}{2} \leq \phi \leq 1$</td>
<td>$\forall \xi$</td>
<td>$\Omega \leq \frac{-\xi + \sqrt{\xi^2 + 2(\phi - \frac{1}{2})}}{\phi - \frac{1}{2}}$</td>
</tr>
<tr>
<td>$\xi \leq \sqrt{2(1 - \phi)}$</td>
<td>$\Omega \leq \frac{-\xi + \sqrt{\xi^2 - 2(1 - \phi)1 - \phi}}{1 - \phi}$</td>
<td>unconditionally</td>
</tr>
<tr>
<td>$\xi &gt; \sqrt{2(1 - \phi)}$</td>
<td>$\Omega \leq \frac{-\xi + \sqrt{\xi^2 - 2(1 - \phi)1 - \phi}}{1 - \phi}$</td>
<td></td>
</tr>
</tbody>
</table>

Figures 3 and 4 show the stability regions for different values of damping coefficient.

### 3.2 Numerical applications

Let us consider a one-dimensional elastic beam of length $L$, Young modulus $E$ and mass per unit volume $\rho$ initially at rest. The right end of the model has an initial velocity $v_0$. The left end boundary condition is fixed. In such a case, the celerity of the longitudinal waves is given by $c = \sqrt{\left(\frac{E}{\rho}\right)}$. An exact solution of the continuous
Figure 3: Stability limit of $\Omega$ in relation with $\phi$. $\xi = 0.5$.

Figure 4: Stability limit of $\Omega$ in relation with $\phi$. $\xi = 1$.

problem can be obtained. The velocity of a section of the beam corresponds to the convolution product between the Dirac function and the initial velocity.

This solution is an harmonic square function with a $T = \frac{2l}{c}$ periodicity. The following figures show the evolution of the position of the right end of the beam as a function of time for the different algorithms presented.

On the different figures, only the wave envelopes are showed to improve data reading.

Figure (5) gives an example of wave representation with upper and lower corresponding envelopes.

Results obtained with Ls-Dyna without any viscosity coefficient closely agree with those calculated by Tchamwa model with $\Phi = 1.01$ for a time step of $0.1 \, t_e$ (cf. figure6).

Variation of the $\Phi$ parameter allows to control the attenuation of high frequencies (figure. 7). For all cases, oscillations disappear from the first up and down
Figure 5: Example of wave representation.

Figure 6: LsDyna and Tchamwa results envelopes

propagation time of the wave on the full bar. However, this result is dependent on time step (figure 8). One can see that the best choice for the time step is close to the critical one. We observe the same phenomena for all other explicit schemes.

In the case of a two element mesh, we note that the three new algorithms lead to the same results, cf. figure (9), that is also the theoretical solution of the discretized problem.
Conclusion

The comparison of the various algorithms shows the intrinsic quality of filtration of the suggested diagrams, in particular the algorithm of Tchamwa-Wielgosz with $\Phi = 1.01$, without any use of classical bulk viscosity. We also showed that attenuation was strongly dependent on the step of time. The more this one is close to the
critical step the more filtering is effective. Of course, as the habitual objective is to be as close as possible to critical time step, this fact often don’t constitute a real limitation. At last due to the whole separation between time and space discretization, these results can be naturally expand to more complex geometries.

References