Algorithms of direct integration of operator DYNA_LINE_TRAN

Summary:

This document describes the diagrams of temporal integration which are used to solve in a direct way of the problems of dynamics in **transitory linear mechanics**. Diagrams of NEWMARK and WILSON θ are detailed, as well as the diagrams “differences centered with constant step” and “pas de adaptive time”.

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1 Introduction

The goal of the transitory dynamic analysis is to determine according to time the answer of a structure, being given an external loading, or boundary conditions the functions of time when the effects of inertia cannot be neglected.

In a certain number of physical configurations, one cannot do without a transitory analysis while being satisfied with a modal or harmonic analysis:

- if the history of the phenomenon has an importance in the study,
- if the external loading is complex (earthquake, excitations multi-components…),
- if the system is nonlinear (plasticity, shocks, friction…).

The methods of analysis transitory dynamics which can be then used are divided into two main categories:

- methods known as of direct integration,
- methods of RITZ including inter alia the recombination of modal projection.

The methods of direct integration are thus called because of fact that no transformation is carried out on the dynamic system after the discretization in finite elements.

We will make a presentation of the algorithms of direct integration used to solve a dynamic problem in mechanics for linear structures. These algorithms are employed in the operator DYNA_LINE_TRAN of *Code_Aster*.

The methods of RITZ, on the contrary, proceed to a transformation of the initial dynamic system, very often a projection on a subspace of the space of starting discretization. The dynamic resolution is done then on a modified system, which gives access only one approximation of the answer of the initial system. They are presented in another document [R5.06.01].

2 Methods of implicit direct temporal integration and clarifies of a dynamic problem

It is supposed that the studied structure has a linear behavior and that the equations governing its dynamic balance were discretized by finished differences or finite elements. One obtains a discrete system of differential equations of the second order which it is a question of integrating in time.

In a general way, these equations take the following shape:

$$\mathbf{M}.\ddot{\mathbf{X}}_t+\mathbf{C}.\dot{\mathbf{X}}_t+\mathbf{K}.\mathbf{X}_t=\mathbf{R}_t$$

- $\mathbf{M}$ is the matrix of mass of the system,
- $\mathbf{C}$ is the matrix of viscous damping of the system,
- $\mathbf{K}$ is the elastic matrix of rigidity of the system,
- $\mathbf{R}$ is the vector of the external forces applied to the viscous system.

The system is of the second order.

Two classes of methods of integration can be distinguished to integrate the equilibrium equations step by step: they are the methods of explicit and implicit integration.

Let us see what distinguishes them by examining temporal integration from the following linear system:

$$\mathbf{M}.\ddot{\mathbf{X}}_t+\mathbf{C}.\dot{\mathbf{X}}_t+\mathbf{K}.\mathbf{X}_t=\mathbf{R}_t$$

This differential connection of the second order can be brought back to a first order system:

$$\mathbf{A}.\dot{\mathbf{u}}=\mathbf{B}.\mathbf{u}+\mathbf{F} \qquad \text{éq 2-1}$$

where:

$$\mathbf{u}=\begin{bmatrix}\mathbf{X}\\ \dot{\mathbf{X}}\end{bmatrix}\ \mathbf{u}=\begin{bmatrix}\dot{\mathbf{X}}\\ \ddot{\mathbf{X}}\end{bmatrix}\ \mathbf{A}=\begin{bmatrix}\mathbf{I} & \mathbf{0}\\ \mathbf{0} & \mathbf{M}\end{bmatrix}\ \mathbf{B}=\begin{bmatrix}\mathbf{0} & \mathbf{I}\\ -\mathbf{K} & -\mathbf{C}\end{bmatrix}\ \mathbf{F}=\begin{bmatrix}\mathbf{0}\\ \mathbf{R}\end{bmatrix}$$

To integrate this differential equation, a discretization is used t_i interval of study as well as a formula of differences finished to express the derivative $\dot{\mathbf{u}}$.

Methods are called **of explicit integration** methods where, in [éq 2-1] written at time t_i , only the derivative $\dot{\mathbf{u}}$ fact of intervening the variable $\mathbf{u}$ at time t_{i+1} . In this way, determination of the sizes sought at the moment t_{i+1} do not result from an inversion of system utilizing the operator $\mathbf{K}$. So moreover, one carries out a “farmhouse-lumping” in order to return the matrix $\mathbf{M}$ diagonal, determination of $\mathbf{u_{i+1}}$ is particularly simple. They are there the main features of the methods of explicit integration.

The implicit or semi-implicit methods utilize the discretization of $\mathbf{U}$ in [éq 2-1] to one posterior moment with t_i , generally t_{i+1} , in order to determine the variables of the problem with t_{i+1} . Their determination thus passes by the resolution of a system utilizing the operator $\mathbf{K}$.

Two concepts concerning the diagrams of integration are important: consistency and stability.

The approximations used to obtain the differential operators define **consistency** or **the order of the diagram of integration**. One can indeed consider that the approximation with which one obtains displacement with each step of time is related to the order of approximation of derived first and seconds compared to time.

The study of **stability** of a diagram consists in analyzing the propagation of the digital disturbances in the course of time. A stable diagram preserves a finished solution, in spite of the disturbances, whereas an unstable diagram led to a digital explosion or divergence of the solution.

To carry out a study of stability of a diagram of integration, one puts this last in the form of a linear recursive system and one determines the particular characteristics of this system. If all the eigenvalues of the operator of recursivity are smaller than 1 modulates some, the diagram is stable, if not it is unstable (cf [bib2]).

The diagrams of integration clarifies are generally conditionally stable, which means that the step of time must be sufficiently small to ensure the stability of the diagram.

Certain implicit algorithms have the characteristic to be unconditionally stable, according to the choice of certain parameters, which makes their interest and makes it possible to integrate the dynamic phenomenon with a step of arbitrarily large time.

The diagram of WILSON θ and the diagram of NEWMARK can be explicit for certain choices of their parameters. In *Code_Aster*, they are employed for their properties of unconditional stability, specific to the implicit schemes. They will thus be classified here in the category of the implicit schemes and one will see under which conditions they give the desired properties of stability.

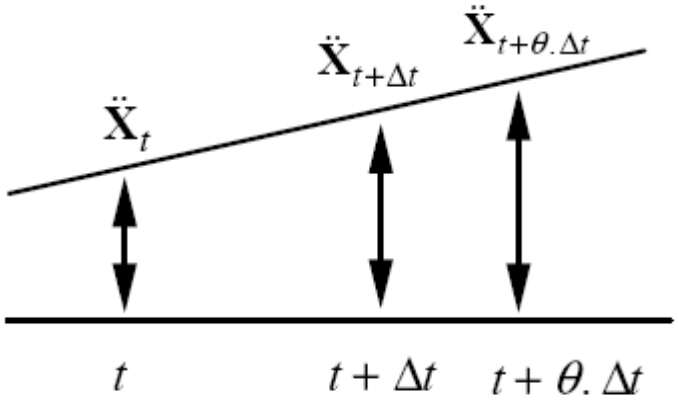
Two explicit diagrams of integration were also introduced into *Code_Aster*. They is the diagrams DIFF_CENTRE and ADAPT who are both based on the method of the centered differences. They are conditionally stable and requires to be powerful a matrix of diagonalized mass. Conditional stability leads to a control of the step of time which, exploited in the case of the diagram ADAPT, allows an adaptation of the step of time according to the speed of the modelled phenomena.

3 The diagram WILSON θ [bib1]

3.1 Presentation of the diagram

It will be supposed in what follows that the solids are elastic linear. This method leaves the assumption that acceleration is linear enters t and $t+\theta.\Delta t$:

$$\ddot{\mathbf{X}}_{t+\tau}=\ddot{\mathbf{X}}_t+\frac{\tau}{\theta.\Delta t}.\left(\ddot{\mathbf{X}}_{t+\theta.\Delta t}-\ddot{\mathbf{X}}_t\right) \quad \text{éq 3.1-1}$$



While integrating [éq 3.1-1] according to the variable t , one obtains:

$$\dot{\mathbf{X}}_{t+\tau}=\dot{\mathbf{X}}_t+\tau\,\ddot{\mathbf{X}}_t+\frac{\tau^2}{2\theta.\Delta t}.\left(\ddot{\mathbf{X}}_{t+\theta.\Delta t}-\ddot{\mathbf{X}}_t\right) \quad \text{éq 3.1-2}$$

$$\mathbf{X}_{t+\tau}=\mathbf{X}_t+\tau\,\dot{\mathbf{X}}_t+\frac{\tau^2}{2}\ddot{\mathbf{X}}+\frac{\tau^3}{6\theta\Delta t}.\left(\ddot{\mathbf{X}}_{t+\theta.\Delta t}-\ddot{\mathbf{X}}_t\right) \quad \text{éq 3.1-3}$$

One writes the equilibrium equations at time $t+\theta.\Delta t$ with $\theta\geq 1$:

$$\mathbf{M}.\ddot{\mathbf{X}}_{t+\theta\Delta t}+\mathbf{C}.\dot{\mathbf{X}}_{t+\theta\Delta t}+\mathbf{K}.\mathbf{X}_{t+\theta\Delta t}=\mathbf{R}_{t+\theta\Delta t} \quad \text{éq 3.1-4}$$

while expressing $\dot{\mathbf{X}}_{t+\theta.\Delta t}$ and $\ddot{\mathbf{X}}_{t+\theta.\Delta t}$ according to $\ddot{\mathbf{X}}_{t+\theta.\Delta t}$ and of $\mathbf{X_t}$, $\dot{\mathbf{X}}_\mathbf{t}$ and $\ddot{\mathbf{X}}_\mathbf{t}$ by the system [éq 3.1 - 2], [éq 3.1-3], and while replacing in [éq 3.1-4], it comes:

$$\tilde{\mathbf{K}}.\mathbf{X}_{\mathbf{t+\theta.\Delta t}}=\tilde{\mathbf{R}}$$

where

$$\tilde{\mathbf{K}}=\mathbf{K}+\frac{3}{(\theta.\Delta t)}.\mathbf{C}+\frac{6}{(\theta.\Delta t)^2}.\mathbf{M}$$

$$\tilde{\mathbf{R}}=\mathbf{R}_t+\theta.\left(\mathbf{R}_{t+\Delta t}-\mathbf{R}_t\right)+\mathbf{M}.\left(a_0.\mathbf{X}_t+a_2.\dot{\mathbf{X}}_t+2.\ddot{\mathbf{X}}_t\right)+\mathbf{C}.\left(a_1.\mathbf{X}_t+2.\dot{\mathbf{X}}_t+a_3.\ddot{\mathbf{X}}_t\right)$$

$$a_0=\frac{6}{(\theta.\Delta t)^2} \qquad a_1=\frac{3}{(\theta.\Delta t)} \qquad a_2=2.a_1 \qquad a_3=\frac{\theta.\Delta t}{2}$$

One goes back to displacements, speeds and accelerations with the step $t+\Delta t$ by the relations:

$$\ddot{\mathbf{X}}_{t+\Delta t}=a_4.\left(\mathbf{X}_{t+\theta.\Delta t}-\mathbf{X}_t\right)+a_5.\dot{\mathbf{X}}_t+a_6.\ddot{\mathbf{X}}_t$$
$$\dot{\mathbf{X}}_{t+\Delta t}=\dot{\mathbf{X}}_t+a_7.\left(\ddot{\mathbf{X}}_{t+\Delta t}+\ddot{\mathbf{X}}_t\right)$$
$$\mathbf{X}_{t+\Delta t}=\mathbf{X}_t+\Delta t\,.\,\dot{\mathbf{X}}_t+a_8.\left(\ddot{\mathbf{X}}_{t+\Delta t}+2\,.\,\ddot{\mathbf{X}}_t\right)$$

$$a_4=\frac{a_0}{\theta}\qquad a_5=\frac{-a_2}{\theta}\qquad a_6=1-\frac{3}{\theta}\qquad a_7=\frac{\Delta t}{2}\qquad a_8=\frac{\Delta t^2}{6}$$

3.2 Complete algorithm of the method WILSON θ :

a) initialization:

1) initial conditions $\mathbf{X_0}, \dot{\mathbf{X}}_0$ and $\ddot{\mathbf{X}}_0$
2) choice of Δt and θ and calculation of the coefficients a_1 ,... a_8 (cf above)
3) to assemble the matrices of rigidity $\mathbf{K}$ and of mass $\mathbf{M}$
4) to form the matrix of effective rigidity $\tilde{\mathbf{K}}=\mathbf{K}+a_0.\mathbf{M}+a_1.\mathbf{C}$
5) to factorize $\tilde{\mathbf{K}}$

b) with each step of time:

1) to calculate the effective loading $\tilde{\mathbf{R}}$
$$\tilde{\mathbf{R}}=\mathbf{R}_t+\theta.\left(\mathbf{R}_{t+\Delta t}-\mathbf{R}_t\right)+\mathbf{M}.\left(a_0.\mathbf{X}_t+a_2.\dot{\mathbf{X}}_t+2.\ddot{\mathbf{X}}_t\right)+\mathbf{C}.\left(a_1.\mathbf{X}_t+2.\dot{\mathbf{X}}_t+a_3.\ddot{\mathbf{X}}_t\right)$$
2) to solve $\tilde{\mathbf{K}}.\mathbf{X}_{t+\theta.\Delta t}=\tilde{\mathbf{R}}$
3) to calculate displacements at time $t+\Delta t$
$$\ddot{\mathbf{X}}_{t+\Delta t}=a_4.\left(\mathbf{X}_{t+\theta.\Delta t}-\mathbf{X}_t\right)+a_5.\dot{\mathbf{X}}_t+a_6.\ddot{\mathbf{X}}_t$$
$$\dot{\mathbf{X}}_{t+\Delta t}=\dot{\mathbf{X}}_t+a_7.\left(\ddot{\mathbf{X}}_{t+\Delta t}+\ddot{\mathbf{X}}_t\right)$$
$$\mathbf{X}_{t+\Delta t}=\mathbf{X}_t+\Delta t\,.\,\dot{\mathbf{X}}_t+a_8.\left(\ddot{\mathbf{X}}_{t+\Delta t}+2.\ddot{\mathbf{X}}_t\right)$$
4) calculation of the step of next time: return to the beginning

3.3 Stability condition of the diagram WILSON θ

The method is unconditionally stable for WILSON θ > 1.37, a value usually employed for θ being 1.4. Moreover, the method presents digital dissipation for $\theta>1$, all the more important as θ increase.

The key word factor `WILSON: (THETA: HT)` allows to specify the use of this algorithm and the choice of the value of θ . By default, the value of θ is taken to 1.4.

4 The diagram of NEWMARK [bib1], [bib2]

4.1 Presentation of the diagram

NEWMARK introduced two parameters γ and β for the calculation positions and speeds to the step $t+\Delta t$:

$$\dot{\mathbf{X}}_{t+\Delta t}=\dot{\mathbf{X}}_t+\Delta t.\left[(1-\gamma).\ddot{\mathbf{X}}_t+\gamma.\ddot{\mathbf{X}}_{t+\Delta t}\right]$$

$$\mathbf{X}_{t+\Delta t}=\mathbf{X}_t+\Delta t.\dot{\mathbf{X}}_t+\Delta t^2.\left[\left(\frac{1}{2}-\beta\right).\ddot{\mathbf{X}}_t+\beta.\ddot{\mathbf{X}}_{t+\Delta t}\right]$$

Let us consider the equilibrium equations at time $t+\Delta t$:

$$\mathbf{M}.\ddot{\mathbf{X}}_{t+\Delta t}+\mathbf{C}.\dot{\mathbf{X}}_{t+\Delta t}+\mathbf{K}.\mathbf{X}_{t+\Delta t}=\mathbf{R}_{t+\Delta t}$$

let us defer the preceding relations while eliminating $\dot{\mathbf{X}}_{t+\Delta t}$ and $\ddot{\mathbf{X}}_{t+\Delta t}$, it comes:

$$\tilde{\mathbf{K}}.\mathbf{X}_{t+\Delta t}=\tilde{\mathbf{R}} \qquad \text{où : } \tilde{\mathbf{K}}=\mathbf{K}+a_0.\mathbf{M}+a_1.\mathbf{C}$$

$$\tilde{\mathbf{R}}=\mathbf{R}_{t+\Delta t}+\mathbf{C}.\left(a_1.\mathbf{X}_t+a_4.\dot{\mathbf{X}}_t+a_5.\ddot{\mathbf{X}}_t\right)+\mathbf{M}.\left(a_0.\mathbf{X}_t+a_2.\dot{\mathbf{X}}_t+a_3.\ddot{\mathbf{X}}_t\right)$$

with:

$$a_0=\frac{1}{(\beta.\Delta t^2)} \qquad a_1=\frac{\gamma}{(\beta.\Delta t)} \qquad a_2=\frac{1}{(\beta.\Delta t)} \qquad a_3=\frac{1}{2\beta}-1$$

$$a_4=\frac{\gamma}{\beta}-1 \qquad a_5=\frac{\Delta t}{2}\left(\frac{\gamma}{\beta}-2\right) \qquad a_6=\Delta t.(1-\gamma) \qquad a_{7}=\gamma.\Delta t$$

4.2 Complete algorithm of the method of NEWMARK

a) initialization:

1) initial conditions $\mathbf{X_0}, \dot{\mathbf{X}}_0$ and $\ddot{\mathbf{X}}_0$
2) choice of Δt and γ , β and calculation of the coefficients a_1 ,... a_8 (cf above)
3) to assemble the matrices of stiffness $\mathbf{K}$ and of mass $\mathbf{M}$
4) to form the matrix of effective rigidity $\tilde{\mathbf{K}}=\mathbf{K}+a_0.\mathbf{M}+a_1.\mathbf{C}$
5) to factorize $\tilde{\mathbf{K}}$

b) with each step of time:

to calculate the effective loading $\tilde{\mathbf{R}}$

2 $\tilde{\mathbf{R}}=\mathbf{R}_{t+\Delta t}+\mathbf{M}.\left(a_0.\mathbf{X}_t+a_2.\dot{\mathbf{X}}_t+a_3.\ddot{\mathbf{X}}_t\right)+\mathbf{C}.\left(a_1.\mathbf{X}_t+a_4.\dot{\mathbf{X}}_t+a_5.\ddot{\mathbf{X}}_t\right)$

to solve $\tilde{\mathbf{K}}.\mathbf{X}_{t+0.\Delta t}=\tilde{\mathbf{R}}$

to calculate speeds and accelerations at time $t+\Delta t$

$$\ddot{\mathbf{X}}_{t+\Delta t}=a_0.\left(\mathbf{X}_{t+\Delta t}-\mathbf{X}_t\right)-a_2.\dot{\mathbf{X}}_t-a_3.\ddot{\mathbf{X}}_t$$

$$\dot{\mathbf{X}}_{t+\Delta t}=\dot{\mathbf{X}}_t+a_6.\ddot{\mathbf{X}}_t+a_7.\ddot{\mathbf{X}}_{t+\Delta t}$$

5 calculation of the step of next time: return to the beginning

4.3 Stability conditions of the diagram of NEWMARK:

The method of NEWMARK is unconditionally stable if:

$$\gamma > 0.5 \quad \text{and} \quad \beta > \frac{(2\gamma+1)^2}{4}$$

One introduces a positive digital damping if $\gamma > 0.5$ and negative if $\gamma < 0.5$. When $\gamma = 0.5$ and $\beta = 0$, the formula of NEWMARK is reduced to the diagram centered differences. A combination very often employed is $\gamma = 0.5$ and $\beta = \frac{1}{4}$, because it leads to a diagram of a nature 2, unconditionally stable without digital damping.

This diagram of integration is used in a rather widespread way in the field of mechanics, because it makes it possible to choose the order of integration, to introduce or not digital damping, and has a very good precision. It is integrated in *Code_Aster* in the operator DYNA_LINE_TRAN. The keyword factor NEWMARK: (BETA: beta, GAMMA: gamm) allows to specify the use of this algorithm and the choice of the value of β and γ. By default, the value of β is taken to 0.25 and the value of γ is taken to 0.5.

5 Digital damping of the implicit schemes

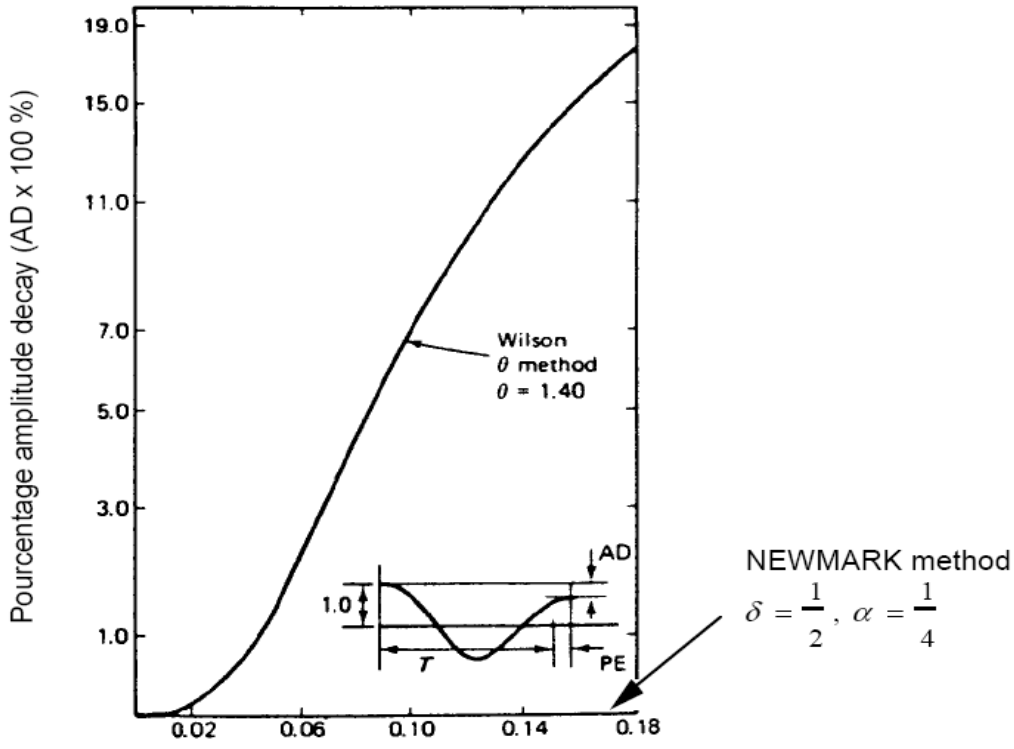
The digital advantage of the direct diagrams of implicit integration lies in the fact that the step of time can be substanciellement large compared to the smallest clean period of the system without being likely to cause an instability of the results.

However, if the contents of the answer reside in a set of clean modes, of which highest an Eigen frequency has F_{max} , one will have to still respect a criterion on the step of time of the form:

$$\Delta t < \frac{1}{(10 * F_{max})} \text{ with } \frac{1}{(100 * F_{max})}$$

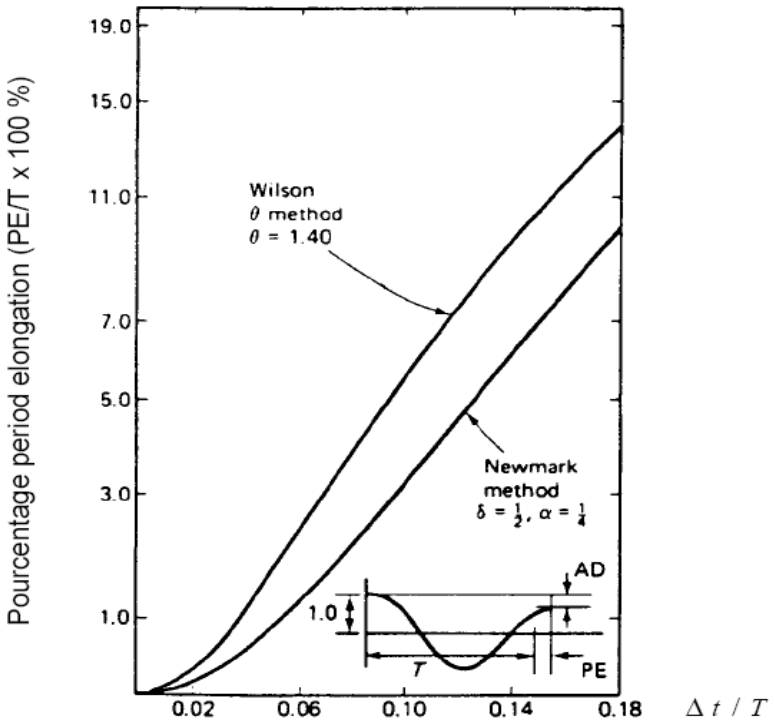
For modes of period clean about the step of time or lower than the step of time, the algorithms of integration introduce a strong damping which contributes to erase the contribution of these high modes.

One can see on the graph hereafter the reduction in amplitude of a system to a degree of freedom, without damping, when one integrates it by various methods (WILSON θ and NEWMARK $\gamma = \frac{1}{2}$, $\beta = \frac{1}{4}$):



It is checked here that the algorithm of NEWMARK with these parameters does not present any digital damping.

On the other hand, the implicit algorithms also have a rather significant effect of elongation of the clean periods contained in the answer of the structure which leads to a dephasing of the calculated solution. The graph below presents percentages of elongation of the clean period of a system to a ddl without damping.



On these 2 graphs, it is noted that to guarantee a precision on the amplitude and the phase of calculated displacements, it is necessary to respect a criterion close to:

$$\Delta t < \frac{0.1}{F_{max}} \text{ à } \frac{0.01}{F_{max}}$$

where F_{max} is the high frequency of the movement which one wishes to correctly capture in the digital analysis.

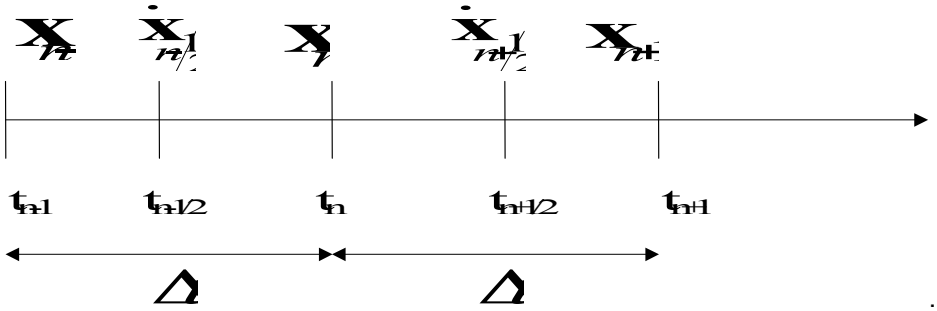
6 Diagram of the centered differences with constant step

6.1 Principle

The diagram clarifies centered differences with constant step is written:

$$\dot{\mathbf{X}}_{n+\frac{1}{2}} = \dot{\mathbf{X}}_{n-\frac{1}{2}} + \Delta t\, \ddot{\mathbf{X}}_n\left(t_n, \mathbf{X}_n, \dot{\mathbf{X}}_n\right) + o\left(\Delta t^2\right)$$
$$\mathbf{X}_{n+1} = \mathbf{X}_n + \Delta t\, \dot{\mathbf{X}}_{n+\frac{1}{2}}\left(t_n, \mathbf{X}_n, \dot{\mathbf{X}}_n\right) + o\left(\Delta t^2\right)$$

with the following notations:



Speed is expressed with indices half-entireties discretization in time whereas displacements and accelerations are expressed with the whole indices.
Written this way, the diagram is of order 2.

Acceleration in t_n is not immediately calculable because speed is known only with the half-not of previous time (in $t_{n-1/2}$), which poses problem to evaluate the terms of damping. To circumvent this difficulty, one calculates acceleration in t_n by the following approximation:

$$\ddot{\mathbf{X}}_n\left(t_n,\mathbf{X}_n,\dot{\mathbf{X}}_n\right)\tilde{=}\ddot{\mathbf{X}}_n\left(t_n,\mathbf{X}_n,\dot{\mathbf{X}}_{n-1/2}\right)=\mathbf{M}^{-1}\left(\mathbf{F}\left(t_n\right)-\mathbf{K}.\mathbf{X}_n-\mathbf{C}.\dot{\mathbf{X}}_{n-1/2}\right)$$

what constitutes a valid approximation if damping is sufficiently weak ($\dot{\mathbf{X}}_n=\dot{\mathbf{X}}_{n-1/2}+o(1)$). The diagram loses its precision of order 2 if the damping of the structure is important.
Other methods of approximation of acceleration can be considered. That selected appeared a good compromise between simplicity and stability, like the study described in the reference [bib4] on the precision and the stability of several methods.

The fields are filed at the moments $t_n, t_{n+1}, \ldots$, speed being approximate at these moments by the following formula:

$$\dot{\mathbf{X}}_{n+1}=\dot{\mathbf{X}}_{n+1/2}+\frac{\Delta t}{2}\ddot{\mathbf{X}}_{n+1}\left(t_{n+1},\mathbf{X}_{n+1},\dot{\mathbf{X}}_{n+1/2}\right)$$

6.2 Stability

The diagram of the centered differences is **conditionally stable**. In the case of a system without damping [bib2], the diagram is stable for a step of checking time $\Delta t<\frac{2}{\omega_{\max}}$ where $\omega_{\max}$ is the greatest own pulsation of the system, that is to say $\Delta t<\frac{T_{\min}}{\pi}$. A minimum of π is needed not time to describe the smallest period of the system $T_{\min}$.
The limiting value for the step of time decreases slowly when damping increases [bib4]. For example, for a damping of 0.5%, the condition becomes $\Delta t<\frac{T_{\min}}{5}$.

6.3 Algorithm

In short, the diagram such as it is introduced into *Code_Aster* presents itself in the following way:

0 inialisation:
Δt , $\mathbf{X}_0$, $\dot{\mathbf{X}}_0$ given
$\ddot{\mathbf{X}}_0=\mathbf{M}^{-1}\left(\mathbf{F}\left(t=0\right)\right)-\mathbf{K}.\mathbf{X}_0-\mathbf{C}.\dot{\mathbf{X}}_0$

$$\dot{\mathbf{X}}_{-1/2}=\dot{\mathbf{X}}_0-\frac{\Delta t}{2}\ddot{\mathbf{X}}_0$$

1 With each step of time $\mathbf{X}_n, \dot{\mathbf{X}}_{n-1/2}, \ddot{\mathbf{X}}_n$ known

$$\dot{\mathbf{X}}_{n+1/2}=\dot{\mathbf{X}}_{n+1/2}+\Delta t\,\ddot{\mathbf{X}}_n\left(t_n,\mathbf{X}_n,\dot{\mathbf{X}}_{n+1/2}\right)$$

$$\mathbf{X}_{n+1}=\mathbf{X}_n+\Delta t\,\dot{\mathbf{X}}_{n+1/2}$$

$$\ddot{\mathbf{X}}_{n+1}=\mathbf{M}^{-1}\left(\mathbf{F}\left(t_n\right)-\mathbf{K}.\mathbf{X}_{n+1}-\mathbf{C}.\dot{\mathbf{X}}_{n-1/2}\right)$$

$$\dot{\mathbf{X}}_{n+1}=\dot{\mathbf{X}}_{n+1/2}+\frac{\Delta t}{2}\ddot{\mathbf{X}}_{n+1}$$

2 possible filing of $\mathbf{X}_{n+1}, \dot{\mathbf{X}}_{n+1}, \ddot{\mathbf{X}}_{n+1}$
then return at the stage 1) for the following step.

6.4 Matrix of diagonal mass

The calculation of acceleration requires the inversion of the matrix of mass. This explicit diagram becomes more performing if one uses a matrix of concentrated mass ('MASS_LUMPING ') so that it is diagonal. The inversion then does not require any more factorization and is immediate.
This is why in *Code_Aster*, the diagram of centered differences is licit only with built matrices of mass in a diagonal way, by the option 'MASS_MECA_DIAG' of the operator CALC_MATR_ELEM.

6.5 Checking of the step of time

It was seen that the diagram of centered differences is stable provided that the step of time, in the absence of damping, that is to say lower than a limiting value, equalizes with $\Delta t<\frac{2}{\omega_{\max}}$. In practice one employs a step of time which is worth from 5% to 20% of the step of critical time. It was thus introduced a test on the step of time which checks that:

$\Delta t<0,05\frac{2\pi}{\max\limits_{1\le i\le nddl}\left(\sqrt{\frac{k_{ii}}{m_{ii}}}\right)}$ where k_{ii} and m_{ii} are the diagonal terms of the matrices of stiffness and mass.
If this condition is not checked, the user is stopped with a message indicating the step of maximum time to him who it can use.

6.6 Calculation of acceleration

The calculation of acceleration is done as follows:
for each degree of freedom, one tests if the diagonal term of the matrix of mass corresponding is null.

- if it is not null, the term of acceleration is calculated according to the formula: $\ddot{\mathbf{X}}_{n+1}=\mathbf{M}^{-1}\left(\mathbf{F}\left(t_n\right)-\mathbf{K}.\mathbf{X}_{n+1}-\mathbf{C}.\dot{\mathbf{X}}_{n-\frac{1}{2}}\right)$
- if it is null, the term of acceleration is not calculated. It is the case for degrees of freedom known as of Lagrange. If they correspond to blocked degrees of freedom, it is licit not to take account of the line in question and not to calculate its acceleration. In case where the degree of freedom of Lagrange was introduced to define a connection between two freedom degrees, that does not have any more a direction. The diagram is thus then unusable and a test stops the execution with an explicit message.

7 Diagram with step of adaptive time

7.1 Principle

The methods of calculating clarifies are particularly indicated in the simulation of fast phenomena, such as the wave propagation in the solids. On the other hand, they agree less better with slower phenomena since the stability condition of the diagram imposes a step of time of about a smallest clean period of the system.

The adaptive diagram, based on the diagram of centered differences, was developed to allow the calculation of transitory answers in which fast" and "slow" phenomena ". For example at the time of an impact, initially of the high frequency waves are propagated and dissipate themselves in the structure. Then, the structure does not answer any more but on its modes of low frequencies, the high frequencies being deadened. The idea is thus to adapt the step of time progressively according to the concerned phenomena, by fixing a criterion of precision on the solution.

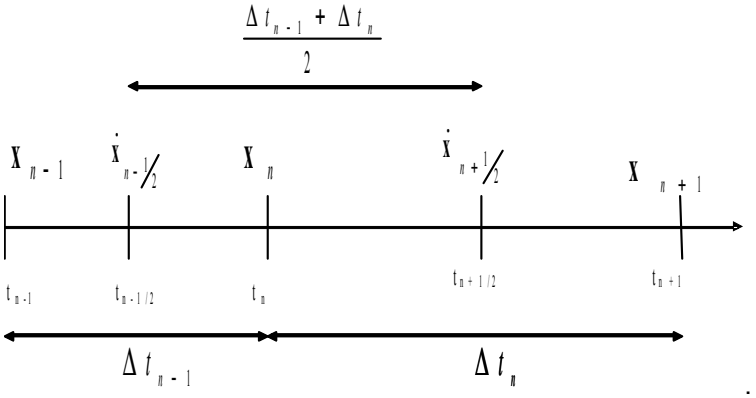
7.2 Diagram

The diagram clarifies centered differences with variable steps is written:

$$\dot{\mathbf{X}}_{n+\frac{1}{2}} = \dot{\mathbf{X}}_{n-\frac{1}{2}} + \frac{\Delta t_{n-1} + \Delta t_n}{2} \ddot{\mathbf{X}}_n\left(t_n, \mathbf{X}_n, \dot{\mathbf{X}}_n\right) + o\left(\Delta t^2\right)$$

$$\mathbf{X}_{n+1} = \mathbf{X}_n + \Delta t\, \dot{\mathbf{X}}_{n+\frac{1}{2}}\left(t_n, \mathbf{X}_n, \dot{\mathbf{X}}_n\right) + o\left(\Delta t^2\right)$$

with the following notations:



It is noted that the step of time varies. It is subscripted: Δt_n .
That has as a consequence which the diagram is not rigorously any more of the second order, since it "is not centered any more". More Δt_{n-1} and Δt_n are different, more the order of the diagram is close to 1. Strong variations of the step of time are thus accompanied by a fall of precision. The formula speed employed leads to good performances when the step of time decreases but cause a drop in the limit of stability when the step of time increases. This is why one it constrained to only increase very gradually.
Lastly, one uses the same approximations as for the differences centered with regard to calculation of accelerations and speeds to the steps of "whole" times:

- acceleration is estimated by $\ddot{\mathbf{X}}_n\left(t_n, \mathbf{X}_n, \dot{\mathbf{X}}_n\right) \tilde{=} \ddot{\mathbf{X}}_n\left(t_n, \mathbf{X}_n, \dot{\mathbf{X}}_{n-\frac{1}{2}}\right)$ and $\ddot{\mathbf{X}}_n\left(t_n, \mathbf{X}_n, \dot{\mathbf{X}}_{n-\frac{1}{2}}\right) = \mathbf{M}^{-1}.\left(\mathbf{F}\left(t_n\right) - \mathbf{K}.\mathbf{X}_n - \mathbf{C}\,\dot{\mathbf{X}}_{n-\frac{1}{2}}\right)$;
- and stored speed is evaluated by $\dot{\mathbf{X}}_{n+1} = \dot{\mathbf{X}}_{n+\frac{1}{2}} + \frac{\Delta t}{2}\ddot{\mathbf{X}}_{n+1}$.

As for the diagram of centered differences, of which it is inspired, the diagram with adaptive step requires the inversion of the matrix of mass. This is why one requires the diagonalisation of the matrix of mass as well as the same restrictions on the degrees of freedom of Lagrange as for the diagram on centered differences.

7.3 Estimate of the step of time according to the precision required

To define a criterion on the step of time according to the precision required on the solution, one introduces the concept of **frequency connects disturbed** [bib4]:

$$f_{AP_n}=\frac{1}{2\pi}\sqrt{\left|\frac{\ddot{X}_x-\ddot{X}_{x-1}}{X_x-X_{x-1}}\right|}$$

This size can be interpreted like the "instantaneous frequency" of the system. It is indeed an approximation of the local slope of the curve forces/displacement. It is related to the error due to truncation in the limited developments of the diagram. It makes it possible moreover to take account of the external forces and their fluctuations in frequency.
In the case of a system with several degrees of freedom, it is necessary to calculate an apparent frequency for each degree of freedom. One then employs the maximum on all the frequencies calculated to determine the step of time.
If the denominator tends towards zero, the apparent frequency can become very large and lose its physical significance. One then obtains an unjustified refinement of the step of time when speed is cancelled. In the case of sinusoidal oscillations, it is the case twice per period. One modifies the criterion then by introducing the following condition:

$$\frac{|X_x-X_{x-1}|}{\Delta t}\leq \dot{X}_{\min}\Rightarrow f_{AP_n}=\frac{1}{2\pi}\sqrt{\left|\frac{\ddot{X}_x-\ddot{X}_{x-1}}{\dot{X}_{\min}\Delta t}\right|}$$

One obtains an intermediary between the frequency connect disturbed and the truncation error. The value of $\dot{X}_{\min}$ is not easy to determine *a priori* and a badly selected value can lead to an artificial moderation of the apparent frequency.
Two methods are proposed.

7.3.1 influences of the close nodes

In the case of a system with several degrees of freedom, one can make use of the information given by $1\leq j\leq nv$ nodes close to the node i :

$$f_{AP_n}=\max_{DX,\,DY,\,DZ,\,DRX,\,DRY,\,DRZ}\left(\max_{1\leq i\leq \text{nb}\,noeud}\frac{1}{2\pi}\sqrt{\left|\frac{\ddot{X}^i_x-\ddot{X}^i_{x-1}}{b^i_n}\right|}\right)$$

where $b^i_n=\Delta t_n\max\left(10^{-15}ms^{-1}\ ,\ \dot{X}^i_{n+1/2}\ ,\ \frac{1}{100}\max_{1\leq j\leq nv}\left(\dot{X}^j_{n+1/2}\right)\right)$

This method requires the census of the nodes close and the estimate "speeds" according to each type of degree of freedom (translation 'DX', 'DY', 'DZ', and possibly rotation 'DRX', DRY' and 'DRZ') for these close nodes.
Method programmed in *Code_Aster* simplify this formula somewhat and consists, for a degree of freedom given, i , to make starting from this position an ascending research and a downward research on the degrees of freedom in their order of classification defined by NUME_DDL. The first two degrees of freedom, k and l , of comparable nature found respectively before and after the degree of freedom i are regarded as the "neighbors". To limit the cost of this technique, research is made once for all at the beginning of transitory calculation and the "neighbors" are recorded in two tables of entireties.
The use of this method is started by the key word VITE_MIN: 'NORM'.

7.3.2 use of information at previous time

One can be also based on the information brought by the steps of previous times to consider speed minimal. One then estimates it by the following formula:

$$\dot{X}_{\min} = \max_{k<n}\left(\frac{|\dot{X}_k^i|}{100}, 10^{-15}\, ms^{-1}\right)$$

One has then:

$$f_{AP_n} = \max_{DX,\,DY,\,DZ,\,DRX,\,DRY,\,DRZ}\left(\max_{1\le i\le \mathrm{nb}\,noeud}\frac{1}{2\pi}\sqrt{\left|\frac{\ddot{X}_x^i - \ddot{X}_{x\text{-}1}^i}{b_n^i}\right|}\right)$$

with $b_n^i = \Delta t_n \max\left(10^{-15}\, ms^{-1}, \dot{X}^i_{n+1/2}, \frac{1}{100}\max_{k<n}\left(\dot{X}_k^j\right)\right)$

This method is engaged by the key word VITE_MIN: 'MAXIMUM'.

This method cannot be employed if speed varies too much during calculation, because in this case one would have with each step:

$$\frac{|X_n - X_{n\text{-}1}|}{\Delta t} \le \dot{X}^i_{\min}$$

7.4 Choice amongst step per apparent period, N

Error analyses and the criteria of stability established for a system with only one degree of freedom (see [bib4]) made it possible to estimate the number of steps N necessary per period connect to obtain a good precision. These tests showed that a minimum of 20 pas per period is necessary. This number is skeletal by the user in the command file thanks to the key word 'NB_POINT_PERIODE'. Its value by default established to 50 leads to a precision on L' temporal integration of about 1 to 2%.
The step of initial time is used like step as maximum time in the absolute: $\Delta t_{mac} = \Delta t_{initial}$. Balanced by a skeletal coefficient by 'PAS_LIMI_RELA', it is used as step of minimal time: $\Delta t_{\min} = PLR * \Delta t_{initial}$

7.5 Heuristics of evolution of the step of time Δt_n

One defines an indicator, known as "error", on the choice of the step of time:

$$erreur = \Delta t_n N f_{AP_n}$$

It is necessary that this indicator is lower than 1 to hope to guarantee a good temporal integration of the smallest clean period. However the adaptive diagram must concomitantly avoid the use of a step of too small time, which would cause a overcost of calculation then, even the appearance of parasitic "noises".
According to the indicator, the algorithm will increase or decrease the step of time. One defines for that two coefficients, CDP , the coefficient of refinement of the step of time (word key 'COEF_DIV_PAS', value by default: 1.334) and CMP , the coefficient of performance of the step time (word key 'COEF_MULT_PAS', value by default: 1.1).

At the time of this search of the step of optimal time, one defines a maximum iteration count of reduction of the step of time, $iter_{max}$, to avoid with the step of time to evolve in a too brutal way, which is prejudicial with the order of the diagram, and not to launch a too expensive optimization.

- if the indicator of error is higher than its limiting value, that one did not exceed the limiting number of refinement for a step of time and that the step of time remains larger than its fixed minimal value *a priori*, the step of time is refined:
$\Delta t_n > \frac{1}{Nf_{AP_n}}$, $iter < iter_{max}$ et $\Delta t_n > \Delta t_{\min} \Rightarrow \frac{\Delta t_n}{CDP} \rightarrow \Delta t_n$,
- if the indicator shows that since five consecutive steps the step of time appears too fine, i.e.
$\Delta t_n < \frac{0,75}{Nf_{AP_n}}$, then $\min\left(\Delta t_{\min}, \mathrm{CMP}\,\Delta t_n\right) \rightarrow \Delta t_n$

7.6 Algorithm

the algorithm was programmed in *Code_Aster* according to the following flow chart:

0 Initialization:

$\mathbf{X_0}$, $\dot{\mathbf{X}}_0$ given

$\ddot{\mathbf{X}}_0 = \mathbf{M}^{-1}\left(\mathbf{F}\left(t=0\right)\right) - \mathbf{K}\,\mathbf{X}_0 - \mathbf{C}\,\dot{\mathbf{X}}_0$

$\dot{\mathbf{X}}_{-1/2} = \dot{\mathbf{X}}_0 - \frac{\Delta t}{2}\ddot{\mathbf{X}}_0$

recovery of the parameters of integration:

$\Delta t_{initial}$

CMP coefficient of performance of the step of time

CDP coefficient of reduction of the step of time

PLR limit with refinement such as $\Delta t \geq PLR\,\Delta t_{initial}$

NR many steps of time per apparent period

$iter_{max}$ maximum number of reductions of the step of time

1 with each step of time:

$\mathbf{X}_n$, $\dot{\mathbf{X}}_{n-1/2}$, $\ddot{\mathbf{X}}_n$ known

$t_{n+1} = t_n + \Delta t_n$

1.0

iter=0

1.1: temporal integration

$\dot{\mathbf{X}}_{n+\frac{1}{2}} = \dot{\mathbf{X}}_{n-\frac{1}{2}} + \frac{\Delta t_{n-1} + \Delta t_n}{2}\ddot{\mathbf{X}}_n$

$\mathbf{X}_{n+1} = \mathbf{X}_n + \Delta t_n\,\dot{\mathbf{X}}_{n+\frac{1}{2}}$

$\ddot{\mathbf{X}}_{n+1} = \mathbf{M}^{-1}.\left(\mathbf{F}\left(t_{n+1}\right) - \mathbf{K}\,.\,\mathbf{X}_{n+1} - \mathbf{C}.\dot{\mathbf{X}}_{n+\frac{1}{2}}\right)$

$\dot{\mathbf{X}}_{n+1} = \dot{\mathbf{X}}_{n+\frac{1}{2}} + \frac{\Delta t_n}{2}\ddot{\mathbf{X}}_{n+1}$

1.2 calculation of the apparent frequency and the error on the step of time

$f_{AP_n} = \max_{DX,\,DY,\,DZ,\,DRX,\,DRY,\,DRZ}\left(\max_{1 \leq i \leq \mathrm{nb}\,noeud} \frac{1}{2\pi}\sqrt{\left|\frac{\ddot{X}^i_x - \ddot{X}^i_{x-1}}{b^i_n}\right|}\right)$

$erreur = \Delta t_n Nf_{AP_n}$

1.2 test on the relevance of the step of time

- if $erreur > 1$ and $iter < iter_{max}$
  then $\Delta t_n / CDP \rightarrow \Delta t_n$
  but yes $\Delta t_n < \Delta t_{\min}$ stop of calculation with error message
  $iter + 1 \rightarrow iter$ and return in 1.1
- if $erreur > 1$ and $iter > iter_{max}$
  then emission of an alarm and passage as in point 2.
- if $erreur < 1$ passage au point 2
  with if $erreur < 0,75$ since 5 pas consecutive:

amplification of the step of time $\Delta t_n = \min\left(\Delta t_{\max}, \mathrm{CMP}\,\Delta t_n\right)$

2 acceptance of the solution: possible filing of $\mathbf{X}_{n+1}, \dot{\mathbf{X}}_{n+1}, \ddot{\mathbf{X}}_{n+1}$
then $n+1 \rightarrow n$: return in 1 for the step of next time

8 Conclusion

the operator DYNA_LINE_TRAN the choice between several methods of temporal integration allows. In their parameter setting by default, the diagrams of WILSON and NEWMARK are unconditionally stable implicit schemes. They thus require a linear inversion of system to each step of time but on the other hand offer a choice of the step time which is restricted only by the smoothness with which one wishes to describe the temporal evolution of the modelled phenomena.

Diagrams DIFF_CENTRE and ADAPT are explicit what avoids to them, in the case of a matrix of diagonal mass, an inversion of expensive matrix. But the conditional stability of this kind of diagram generally leads to the use of small steps of times, conditioned by the smallest clean period of the system. It is thus not guaranteed that the explicit diagrams are systematically faster. That depends on the simulated phenomena. If the physics of these phenomena requires a fine temporal discretization, the step of time employed is naturally in the interval of stability. In the contrary case, the constraints of digital stability involves an inflation in the number of steps of time very expensive.

The diagram ADAPT profitable make information on the frequential contents of the answer to adapt the step of time. The discretization of time is not thus imposed any more by the smallest clean period of the system but by its answer. That can be an advantage when the frequency of the answer evolves in time, like in the case of the impacts.

9 Bibliography

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10 Description of the versions of the document

Version Aster	Author (S) Organization (S)	Description of the modifications
6	*E. BOYERE, G. JACQUART, LIGHT A.C.,* EDF-R&D/AMA, Industrie/CNPE EDF-Pole of Tricastin, EDF-R&D/TESE	Initial text