Algorithms of direct integration of operator DYNA_LINE_TRAN

Summarized:

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**. The diagrams of NEWMARK and WILSON θ are detailed, as well as the diagrams “central differences with step constant” and “time step adaptive”.

Contents

1 Introduction

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

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

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

The methods of analysis transient 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 integration methods direct 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 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 response of the initial system. They are presented in another document [R5.06.01].

2 Integration methods temporal direct implicit and explicit of a dynamic problem

It is supposed that the studied structure has a linear behavior and that the equations governing its dynamic equilibrium were discretized by finite 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 mass matrix of the system,
- $\mathbf{C}$ is the viscous damping matrix of the system,
- $\mathbf{K}$ is the elastic stiffness matrix 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 integration methods can be distinguished to integrate the balance equations step by step: they are the integration methods explicit and implicit.

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:

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

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

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

The implicit or semi-implicit methods utilize the discretization of $\mathbf{U}$ in [éq 2-1] to one posterior time with t_i , generally t_{i+1} , in order to determining 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 notions concerning the diagrams of integration are important: consistency and stability.

The approximations used to obtain the differential operators define **the consistency** or **the order of the diagram of integration**. One can indeed consider that the approximation with which one obtains displacement with each time step 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 numerical 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 numerical 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 recursion 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 time step 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 one time step arbitrarily large.

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.

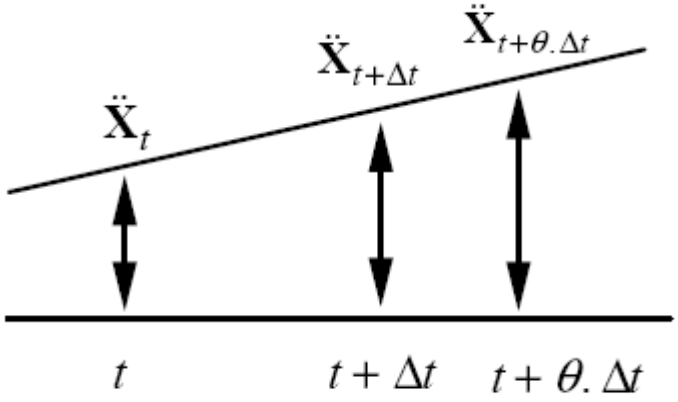
Two explicit diagrams of integration were also introduced into *Code_Aster*. They is diagrams DIFF_CENTRE and ADAPT which are both based on the method of the central differences. They are conditionally stable and requires to be powerful a diagonalized mass matrix. Conditional stability leads to a control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

3 The diagram WILSON θ [bib1]

3.1 Presentation of the diagram

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

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



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

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

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

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

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

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 $\mathbf{X}_{\mathbf{t}}$, $\dot{\mathbf{X}}_{\mathbf{t}}$ 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

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

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

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

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

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

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

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 computation of the coefficients a_1 ,... a_8 (cf above)
3) to assemble the stiffness matrixes $\mathbf{K}$ and mass $\mathbf{M}$
4) to form the effective stiffness matrix $\tilde{\mathbf{K}}=\mathbf{K}+a_0.\mathbf{M}+a_1.\mathbf{C}$
5) to factorize $\tilde{\mathbf{K}}$

b) with each time step:

1) to calculate the effective loading $\tilde{\mathbf{R}}$
   $R=R_t+q.\left(R_{t+Dt}-R_t\right)+M.\left(a_0.X_t+a_2.\dot{X}_t+2.\ddot{X}_t\right)+C.\left(a_1.X_t+2.\dot{X}_t+a\right.$
2) to solve $\tilde{\mathbf{K}}.\mathbf{X}_{\mathbf{t+\theta.\Delta t}}=\tilde{\mathbf{R}}$
3) to calculate displacements at time $t+\Delta t$
   $$\ddot{\mathbf{X}}_{t+\Delta t}=a_4.\left(\mathbf{X}_{\mathbf{t+\theta.\Delta t}}-\mathbf{X}_{\mathbf{t}}\right)+a_5.\dot{\mathbf{X}}_t+a_6.\ddot{\mathbf{X}}_t$$
   $$\dot{\mathbf{X}}_{t+\Delta t}=\dot{\mathbf{X}}_t+a_7.\left(\ddot{\mathbf{X}}_{t+\Delta t}+\ddot{\mathbf{X}}_t\right)$$
   $$\mathbf{X}_{\mathbf{t+\Delta t}}=\mathbf{X}_{\mathbf{t}}+\Delta t.\dot{\mathbf{X}}_t+a_8.\left(\ddot{\mathbf{X}}_{t+\Delta t}+2.\ddot{\mathbf{X}}_t\right)$$
4) computation of time step according to: return to the Stability condition

3.3 beginning 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, method present of numerical dissipation for $\theta>1$, all the more important as θ increases.

The key key factor `WILSON: (THETA: HT)` makes it possible 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 diagram

NEWMARK introduced two parameters γ and β for the computation positions and velocities 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 balance 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:

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

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

with:

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

$$a_4=\frac{\gamma}{\beta}-1 \qquad a_5=\frac{\Delta t}{2}\left(\frac{\gamma}{\beta}-2\right) \qquad a_6=\Delta t.(1-\gamma) \qquad a_{z7}=\gamma.\Delta t$$

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 computation of the coefficients a_1 ,... a_8 (cf above)
3) to assemble the stiffness matrixes $\mathbf{K}$ and mass $\mathbf{M}$
4) to form the effective stiffness matrix $\tilde{\mathbf{K}}=\mathbf{K}+a_0.\mathbf{M}+a_1.\mathbf{C}$
5) to factorize $\tilde{\mathbf{K}}$

b) with each time step:

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

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

to solve $\tilde{\mathbf{K}}.\mathbf{X_{t+\theta.\Delta t}}=\tilde{\mathbf{R}}$

calculate the velocities and accelerations at times $t+\Delta t$

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

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

5 computation of time step according to: return to the Stability conditions

4.3 beginning 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 numerical damping positive 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 central 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 numerical damping.

This diagram of integration is used in a rather widespread way in the field of the mechanics, because it makes it possible to choose the order of integration, to introduce or not numerical damping, and has a very good accuracy. It is integrated in *the Code_Aster* in operator DYNA_LINE_TRAN. The factor key word NEWMARK: (BETA: beta, GAMMA: gamm) makes it possible 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 with 0.25 and the value of γ is taken with 0.5.

5 Numerical damping of the implicit schemes

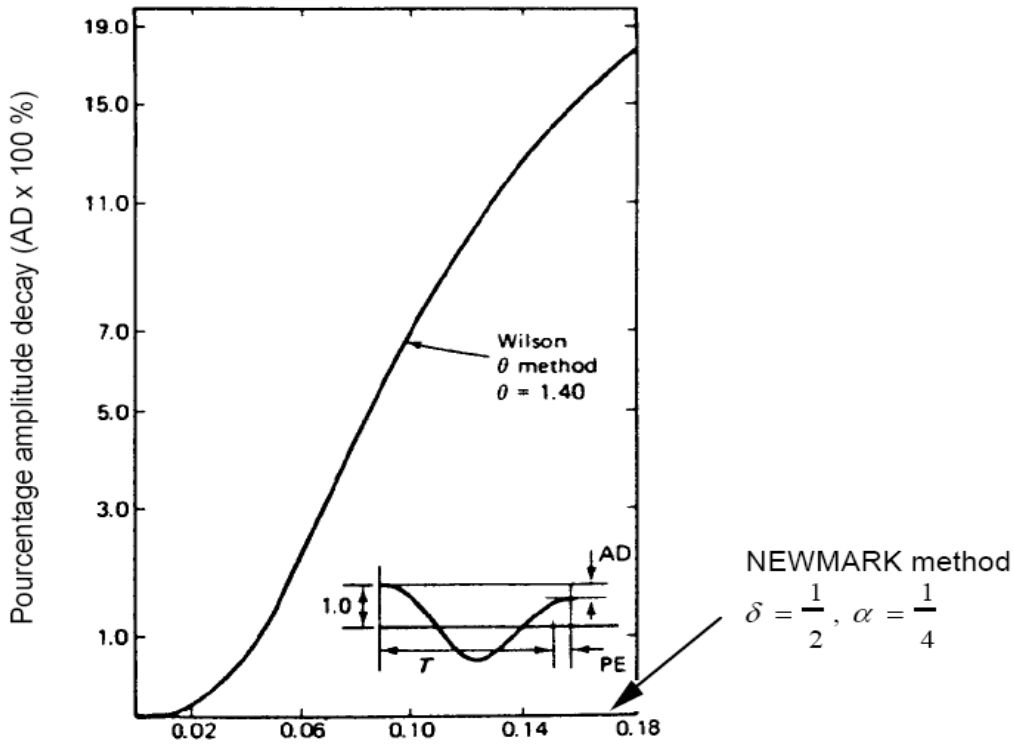
the numerical advantage of the direct diagrams of implicit integration lies in the fact that time step can be substanciellement large compared to the smaller clean period of the system without being likely to cause an instability of the results.

However, if the contents of the response reside in a set of eigen modes, of which highest an eigenfrequency has F_{max}, one must still respect a criterion on time step of the form:

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

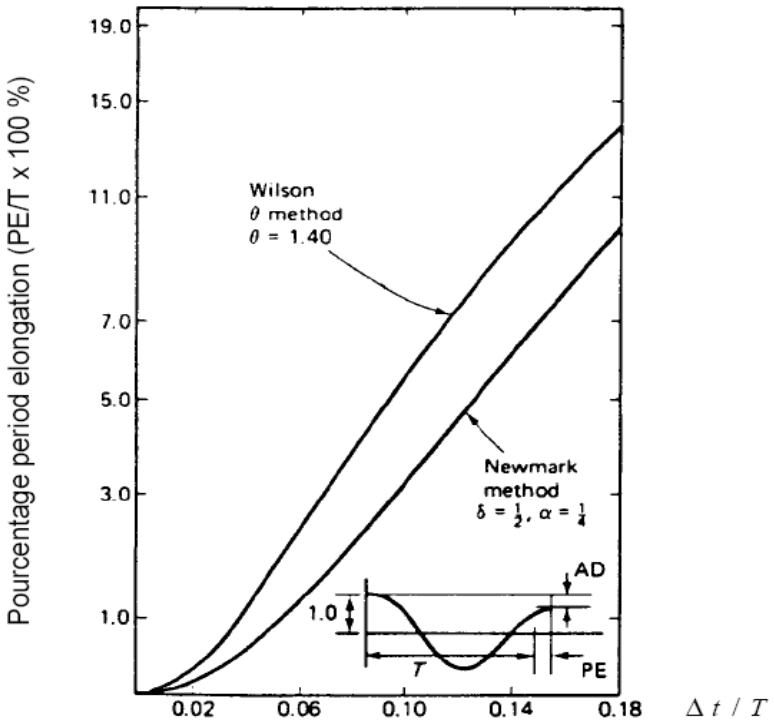
For modes of period clean about time step or lower than time step, the algorithms of integration introduce a strong damping which contributes to erase the contribution of these high modes.

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 numerical damping.

On the other hand, the implicit algorithms also have a rather significant effect of elongation of the clean periods contained in the response of the structure which leads to a phase shift of the calculated solution. The graph below presents percentages of elongation of the clean period of a system to a d.o.f. without damping.



On these 2 graphs, it is noted that to guarantee an accuracy 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 motion which one wishes to correctly capture in the numerical analysis.

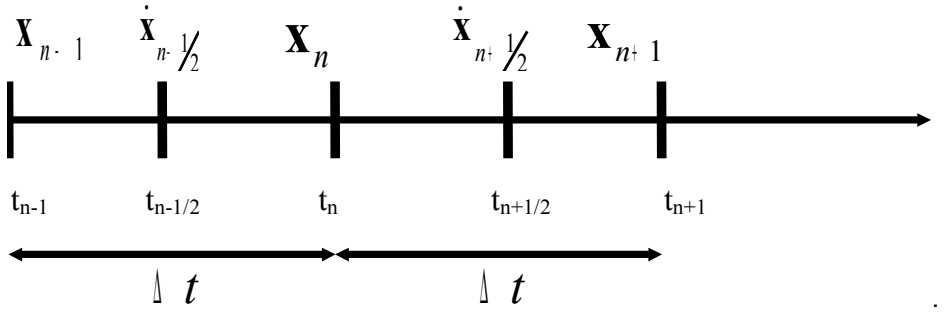
6 Diagram of the central differences with step constant

6.1 Principle

the diagram clarifies central 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:



The velocity is expressed with indices half-integers of the 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 computable because the velocity is known only at the half-PAS 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 L "approximation following:

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

what constitutes a valid approximation if L" damping is sufficiently weak ($\dot{\mathbf{X}}_n=\dot{\mathbf{X}}_{n-1/2}+o(1)$). The diagram loses its accuracy of order 2 if the damping of 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 accuracy and the stability of several methods.

The fields are filed at times $t_n, t_{;+1}, \ldots$, the velocity being approximate at these times 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 central differences is **conditionally stable**. In the case of a system without damping [bib2], the diagram is stable for one time step checking $\Delta t<\frac{2}{\omega_{\max}}$ where $\omega_{\max}$ is the greatest own pulsation of the system, that is to say $\Delta t<\frac{T_{\min}}{\pi}$. Is needed a minimum of π time step to describe the smallest period of the system $T_{\min}$.
The limiting value for time step 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 *the Code_Aster* is presented 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 A each time step $\mathbf{X_n}, \dot{\mathbf{X}}_{n-1/2}, \ddot{\mathbf{X}}_n$ known

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

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

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

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

2 possible archivage 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 Diagonal mass matrix

The computation of acceleration requires the inversion of the mass matrix. This explicit diagram becomes more powerful if one uses a concentrated mass matrix ("MASS_LUMPING ") of such kind qu" it is diagonal. The inversion then does not require any more factorization and is immediate.
This is why in *Code_Aster*, the diagram of central differences is licit only with built mass matrixes in a diagonal way, by option "MASS_MECA_DIAG" of operator CALC_MATR_ELEM.

6.5 Checking of time step

One saw that the diagram of central differences is stable provided that time step, 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 time step who is worth from 5% to 20% of time step criticizes. It was thus introduced a test on time step 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 stiffness matrixes and mass.
If this condition is not checked, the user is stopped with a message indicating the time step maximum one to him that it can use.

6.6 Computation of the acceleration

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

- if it is not null, the term of acceleration is calculated according to the formula: $\ddot{\mathbf{X}}_{n+1}=\mathbf{M}^{-1}\left(\mathbf{F}\left(t_n\right)-\boldsymbol{K}\,\mathbf{X}_{n+1}-\mathbf{C}\,\dot{\mathbf{X}}_{n-1/2}\right)$
- 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 line in question and not to calculate its acceleration. If the degree of freedom of Lagrange were introduced to define a connection between two freedom degrees, that does not have any more a meaning. The diagram is thus then unusable and a test stops the execution with an explicit message.

7 Diagram with time step adaptive

7.1 Principle

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

The adaptive diagram, based on the diagram of central differences, was developed to allow the computation of transient responses in which fast" and "slow" phenomena ". For example during an impact, initially of the high frequency waves are propagated and are dissipated in 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 time step progressively according to the concerned phenomena, by fixing a criterion of accuracy on the solution.

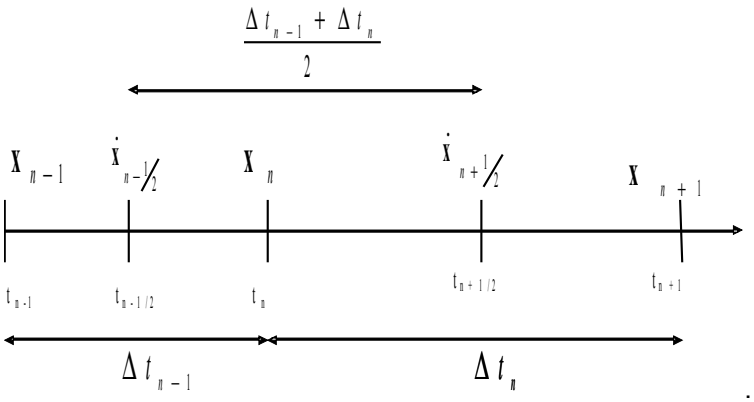
7.2 Diagram

the diagram clarifies central 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 time step 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 time step are thus accompanied by a fall of accuracy. The formula used velocity leads to good performances when time step decreases but cause a drop in the limit of stability when time step increases. This is why one it constrained to only increase very gradually.
Lastly, one uses the same approximations as for the central differences with regard to the computation of accelerations and velocities to time step "whole":

- 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 $\ddot{\mathbf{X}}_n\left(t_n, \mathbf{X_n}, \dot{\mathbf{X}}_{n-\frac{1}{2}}\right) = \mathbf{M}^{-1}\left(\mathbf{F}\left(t_n\right) - \boldsymbol{K}\,\mathbf{X_n} - \mathbf{C}\,\dot{\mathbf{X}}_{n-\frac{1}{2}}\right)$;
- and the stored velocity is evaluated par. $\dot{\mathbf{X}}_{n+1} = \dot{\mathbf{X}}_{n+\frac{1}{2}} + \frac{\Delta t}{2}\ddot{\mathbf{X}}_{n+1}$

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

7.3 Estimate of time step according to the accuracy required

to define a criterion on time step according to the accuracy required on the solution, one introduces the notion of **frequency connect disturbed** [bib4]:

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

This quantity 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 restricted 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 time step.
If the denominator tends towards zero, the apparent frequency can become very large and lose its physical meaning. One then obtains an unjustified refinement of time step when the velocity 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:

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

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 $1\leq j\leq nv$ the nodes close to the node is outside the field of definition with a right profile of the EXCLU type node: i

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

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 "velocities" according to each type of degree of freedom (translation "DX", "DY", "DZ", and possibly rotation "DRX", DRY' and "DRZ") for these close nodes.
The method programmed in *Code_Aster* simplifies this formula somewhat and consists, for a given degree of freedom i, to make from this position an ascending search and a downward search 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 respectively found before and after the degree of freedom i are regarded as the "neighbors". To limit the cost of this technique, the search is made once for all at the beginning of transient computation and the "close" are recorded in two tables of integers.

The use of this method is started by key key VITE_MIN: "NORM".

7.3.2 use of information at previous time

One can also lean on the information brought by the time step preceding ones to consider the velocity 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:

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

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 key key VITE_MIN: "MAXI".

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

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

7.4 Choices amongst step per apparent period, N

analyses error 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 apparent period to obtain a good accuracy. These tests showed that a minimum of 20 steps per period are necessary. This number is skeletal by L `user in the command file thanks to key key "NB_POINT_PERIODE". Its value by default established to 50 leads to an accuracy on temporal integration of about 1 to 2%.
The time step initial one is useful like time step maximum in the absolute: $\Delta t_{mac} = \Delta t_{initial}$. Balanced by a skeletal coefficient by "PAS_LIMI_RELA", it serves as time step minimal: $\Delta t_{\min} = PLR * \Delta t_{initial}$

7.5 Heuristics of evolution of time step Δt_n

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

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

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 time step too small, which would cause a overcost of computation then, even appearance of parasitic "noises".
According to the indicator, the algorithm will increase or decrease time step. One defines for that two coefficients CDP , the coefficient of refinement of time step (key key "COEF_DIV_PAS", value by default: 1,334) and CMP , the coefficient D "amplification of the step time (key key "COEF_MULT_PAS", default value: 1,1).

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

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

7.6

the algorithm were programmed in Code_Aster *according to* the following flow chart: 0

Initiali : given
zation $\mathbf{X_0}, \dot{\mathbf{X}}_0$ recovery

$$\ddot{\mathbf{X}}_0 = \mathbf{M}^{-1}\left(\mathbf{F}(t=0)\right) - \mathbf{K}\,\mathbf{X_0} - \mathbf{C}\,\dot{\mathbf{X}}_0$$

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

of the parameters of integration: CMP
$\Delta t_{initial}$
coefficient of performance of time step the CDP
coefficient of reduction of time step the PLR
limits to refinement such as N $\Delta t \geq PLR\,\Delta t_{initial}$
number of time step per period connect time step
itermax maximum number of reductions from the 1

with each time step: known
$\mathbf{X_n}, \dot{\mathbf{X}}_{n-1/2}, \ddot{\mathbf{X}}_n$ 1.0
$t_{n+1} = t_n + \Delta t_n$
iter
=0 1.1
: temporal integration 1.2

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

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

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

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

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

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

$$erreur = \Delta t_n \, Nf_{AP_n}$$

test on the relevance of time step if

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

from time step the 2 $\Delta t_n = \min\left(\Delta t_{\max}, \text{CMP}\,\Delta t_n\right)$

accep tance of the solution: possible archivage of then $\mathbf{X_{n+1}}, \dot{\mathbf{X}}_{n+1}, \ddot{\mathbf{X}}_{n+1}$
: $n+1 \rightarrow n$ return in 1 for time step according to Conclusion

8

operator DYNA_LINE_TRAN allows the choice between several integration methods temporal. 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 time step 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 diagonal mass matrix, an inversion of expensive matrix. But the conditional stability of this kind of diagram generally leads to the use of small time step, 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, time step employed is naturally in the interval of stability. In the contrary case, the stresses of numerical stability time step involves an inflation in the number of very expensive.

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

9 K.

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