

## Elastodynamics : From Semi - Discrete to Fully Discrete

Assuming that our system exhibits viscous damping, our discrete equations of motion take the following form:

$$\underline{\underline{M}} \ddot{\underline{d}}(t) + \underline{\underline{C}} \dot{\underline{d}}(t) + \underline{\underline{K}} \underline{d}(t) = \underline{F}(t), \quad t \in (0, T)$$

$$\underline{d}(0) = \underline{d}_0$$

$$\dot{\underline{d}}(0) = \dot{\underline{d}}_0$$

There are many techniques for solving the above semi-discrete system. We focus on two classes of techniques : (i) the Newmark method and (ii) the HHT- $\alpha$  method.

### The Newmark Method:

Suppose that we know the solution at time  $t_n$  and seek to find the solution at time  $t_{n+1}$ . Let us define a time-step size  $\Delta t = t_{n+1} - t_n$ , and let us suppose that  $\underline{a}_{n+1} \approx \ddot{\underline{d}}(t_{n+1})$ ,  $\underline{v}_{n+1} \approx \dot{\underline{d}}(t_{n+1})$ , and  $\underline{d}_{n+1} \approx \underline{d}(t_{n+1})$ . Then, a Taylor series expansion of the displacement and velocity vectors suggest the following approximations for  $\underline{v}_{n+1}$  and  $\underline{d}_{n+1}$ :

$$\underline{d}_{n+1} = \underline{d}_n + \Delta t \underline{v}_n + \frac{(\Delta t)^2}{2} ((1-2\beta)\underline{a}_n + 2\beta \underline{a}_{n+1})$$

$$\underline{v}_{n+1} = \underline{v}_n + \Delta t ((1-\gamma)\underline{a}_n + \gamma \underline{a}_{n+1})$$

The above are known as the Newmark formulas, and if the acceleration vector  $\underline{a}_{n+1}$  is known, they yield the displacement vector  $\underline{d}_{n+1}$  and velocity vector  $\underline{v}_{n+1}$ . To close the system, we solve the equations of motion at time  $t_{n+1}$ :

$$\underline{\underline{M}} \underline{a}_{n+1} + \underline{\underline{C}} \underline{v}_{n+1} + \underline{\underline{K}} \underline{d}_{n+1} = \underline{F}_{n+1}$$

Collecting the above relations, we obtain the classical Newmark method:

Classical  
Newmark  
Method

$$\boxed{\begin{aligned} \underline{\underline{M}} \underline{a}_{n+1} + \underline{\underline{C}} \underline{v}_{n+1} + \underline{\underline{K}} \underline{d}_{n+1} &= \underline{F}_{n+1} \\ \underline{d}_{n+1} &= \underline{d}_n + \Delta t \underline{v}_n + \frac{(\Delta t)^2}{2} ((1-2\beta)\underline{a}_n + 2\beta \underline{a}_{n+1}) \\ \underline{v}_{n+1} &= \underline{v}_n + \Delta t ((1-\gamma)\underline{a}_n + \gamma \underline{a}_{n+1}) \end{aligned}}$$

The particular choices of the parameters  $\beta$  and  $\gamma$  determine the properties of the method: for example,  $2\beta \geq \gamma \geq \frac{1}{2}$  achieves unconditional stability and  $\gamma = \frac{1}{2}$  achieves second-order accuracy. In the undamped setting, the stability conditions for the Newmark method are as follows:

$$\text{Unconditional Stability: } 2\beta \geq \gamma \geq \frac{1}{2}$$

$$\text{Conditional Stability: } \gamma \geq \frac{1}{2}$$

$$B < \frac{\gamma}{2}$$

$$\omega^h \Delta t \leq \omega_{\text{crit.}} = (\gamma/2 - B)^{-1/2}$$

$\uparrow$   
Critical Sampling Frequency

The above stability conditions must be satisfied for each mode in the system, so the maximum natural frequency,  $\omega_{\text{max}}$ , is critical and must satisfy  $\omega_{\text{max}} \Delta t \leq \omega_{\text{crit.}}$ . It should be noted that damping acts to increase  $\omega_{\text{crit.}}$ , so the above conditions are conservative in the damped case.

A table listing properties of well-known members of the Newmark family is provided below:

Method	Type	B	$\gamma$	Stability	Accuracy
Trapezoidal Rule (Avg. Acceleration)	Implicit	$\frac{1}{4}$	$\frac{1}{2}$	Unconditional	2
Linear Acceleration	Implicit	$\frac{1}{6}$	$\frac{1}{2}$	$\omega_{\text{crit.}} = 2\sqrt{3}$	2
Fox-Goodwin (Royal Road)	Implicit	$\frac{1}{12}$	$\frac{1}{2}$	$\omega_{\text{crit.}} = \sqrt{6}$	2
Central Difference	Explicit	0	$\frac{1}{2}$	$\omega_{\text{crit.}} = 2$	2

One advantageous property of the Newmark method is that  $B$  and  $\gamma$  may be tuned in order to damp unphysical high-frequency behavior due to spatial discretization. While this is not necessarily required for isogeometric discretizations, it is crucial for guaranteeing accurate and stable long-time integration for classical finite elements. Unfortunately, in terms of the Newmark method,  $\gamma > \frac{1}{2}$  is necessary to introduce high-frequency dissipation, limiting the accuracy of the method to first-order. The MHHT- $\alpha$  method is a generalization of the Newmark method which permits high-frequency dissipation while maintaining second-order accuracy.

For a fixed  $\gamma > \frac{1}{2}$ , one can select  $B$  such that high-frequency dissipation is maximized. This ideal  $B$  is  $B = (\gamma + \frac{1}{2})^2/4$ , and the larger the  $B$  in the range  $\gamma/2 < B < (\gamma + \frac{1}{2})^2/4$ , the greater the dissipation.

In practice, the Newmark equations are not solved exactly but rather a predictor-multicorrector algorithm is employed. At the beginning of each time step, we set the iteration counter to  $i = 0$  and enter a predictor phase where we initialize the approximations as:

$$\dot{\underline{d}}_{n+1}^i = \underline{\dot{d}}_{n+1}, \quad \dot{\underline{v}}_{n+1}^i = \underline{\dot{v}}_{n+1}, \quad \dot{\underline{a}}_{n+1}^i = \underline{\dot{a}}_{n+1}$$

The predictors may be chosen in any way such that they satisfy the Newmark formulas:

$$\hat{d}_{n+1} = d_n + \Delta t \hat{v}_n + \frac{(\Delta t)^2}{2} ((1-2\beta) \hat{a}_n + 2\beta \hat{a}_{n+1})$$

$$\hat{v}_{n+1} = v_n + \Delta t ((1-\gamma) \hat{a}_n + \gamma \hat{a}_{n+1})$$

Typical choices include:

Constant Displacement Predictor: \* Often preferred in Nonlinear Solid Mechanics\*

$$\hat{d}_{n+1} = d_n$$

$$\hat{a}_{n+1} = -\frac{1}{\beta \Delta t} \hat{v}_n - \frac{(1-2\beta)}{2\beta} \hat{a}_n$$

$\hat{v}_{n+1}$  defined by Newmark formula

Constant Velocity Predictor: \* Often preferred in Fluid Mechanics & FSI\*

$$\hat{v}_{n+1} = v_n$$

$$\hat{a}_{n+1} = -\frac{(1-\gamma)}{\gamma} \hat{a}_n$$

$\hat{d}_{n+1}$  defined by Newmark formula

Zero Acceleration Predictor: \* Often used for linear problems\*

$$\hat{a}_{n+1} = 0$$

$$\left. \begin{array}{l} \hat{v}_{n+1} \\ \hat{d}_{n+1} \end{array} \right\} \text{defined by Newmark formulas}$$

We use the  $i^{th}$  values to compute a residual as:

$$\Delta \underline{F}_{n+1}^i = \underline{F}_{n+1} - \underline{M} \hat{a}_{n+1}^i - \underline{C} \hat{v}_{n+1}^i - \underline{K} \hat{d}_{n+1}^i$$

and then use this residual to calculate a correction to the acceleration term by solving:

$$\underline{M}^* \Delta \underline{a} = \Delta \underline{F}_{n+1}^i$$

and once we have solved for  $\Delta \underline{a}$  we enter a corrector phase in which we update the solution:

$$\hat{a}_{n+1}^{i+1} = \hat{a}_{n+1}^i + \Delta \underline{a}$$

$$\hat{v}_{n+1}^{i+1} = \hat{v}_{n+1}^i + \gamma \Delta t \Delta \underline{a}$$

$$\hat{d}_{n+1}^{i+1} = \hat{d}_{n+1}^i + \beta (\Delta t)^2 \Delta \underline{a}$$

The matrix  $\underline{\underline{M}}^*$  depends on the exact method used. If we choose:

$$\underline{\underline{M}}^* = \underline{\underline{M}} + \gamma \Delta t \underline{\underline{C}} + B(\Delta t)^2 \underline{\underline{K}}$$

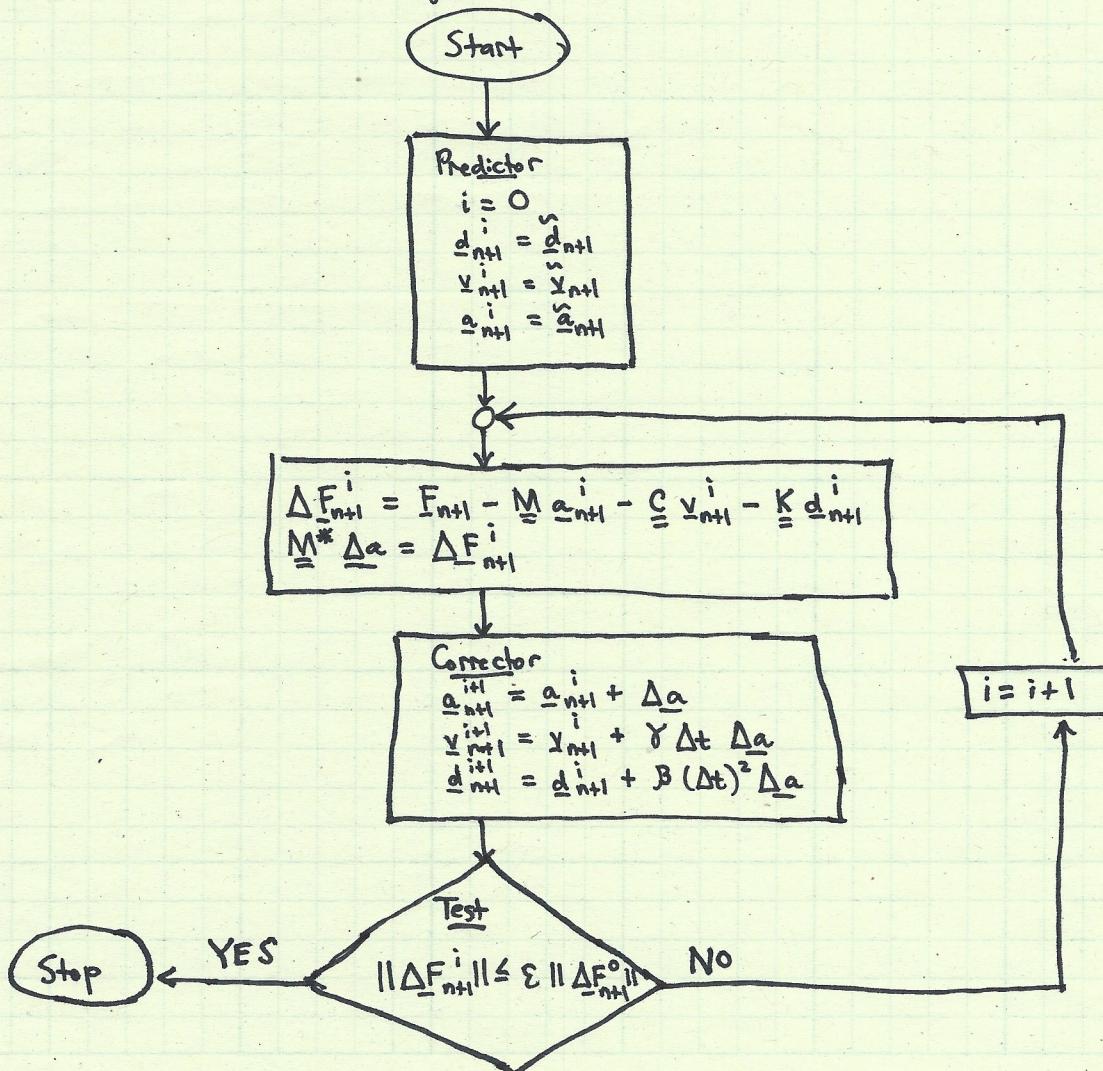
the predictor - multi corrector algorithm converges after one step. However, the resulting matrix system for the acceleration term may be quite expensive to solve. Alternatively, we may choose:

$$\underline{\underline{M}}^* = \underline{\underline{M}}$$

where  $\underline{\underline{M}}$  is the so-called lumped mass matrix whose diagonal components are row sums. The resulting matrix system is trivial to solve, but several corrector steps may be needed for convergence.

At the end of the corrector phase, we check the residual for convergence. If we have that  $\|\underline{\underline{\Delta F}}_{n+1}^i\| \leq \epsilon \|\underline{\underline{\Delta F}}_{n+1}^0\|$  for some predetermined tolerance  $\epsilon$ , we move on to the next time step. If not, we increment the iteration counter  $i$  by 1. It should be noted that even if the exact  $\underline{\underline{M}}^*$  is used, if an inexact linear solver is employed, additional corrector steps may need to be performed.

The full predictor- multi corrector algorithm is summarized in the following algorithm:



### The HHT- $\alpha$ Method:

As previously mentioned, the Newmark algorithm is unable to possess high-frequency dissipation without sacrificing second-order accuracy. For this reason, Hilber, Hughes, and Taylor developed the HHT- $\alpha$  method in:

H.M. Hilber, T.J.R. Hughes, and R.L. Taylor, "Improved numerical dissipation for time integration algorithms in structural dynamics," *Earthquake Engineering and Structural Dynamics*, 5: 283-292. (1977)

The basis of the HHT- $\alpha$  method is to replace the equation of motion in Newmark's method by:

$$\underline{\underline{M}} \underline{\underline{a}}_{n+1} + \underline{\underline{C}} \underline{\underline{v}}_{n+\alpha} + \underline{\underline{K}} \underline{\underline{d}}_{n+\alpha} = \underline{\underline{F}}_{n+1}$$

where:

$$\underline{\underline{v}}_{n+\alpha} = (1-\alpha) \underline{\underline{v}}_n + \alpha \underline{\underline{v}}_{n+1}$$

$$\underline{\underline{d}}_{n+\alpha} = (1-\alpha) \underline{\underline{d}}_n + \alpha \underline{\underline{d}}_{n+1}$$

and  $\alpha$  is a tunable parameter. Hiller, Hughes, and Taylor showed the method is both second-order accurate and unconditionally stable when:

$$\frac{2}{3} \leq \alpha \leq 1$$

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

$$\gamma = \frac{3}{2} - \alpha$$

The HHT- $\alpha$  method defaults to the standard Newmark method when  $\alpha = 1$  and the method possesses high-frequency dissipation when  $\alpha < 1$ . Moreover, the smaller the  $\alpha$ , the greater the dissipation.

The HHT- $\alpha$  method is one of the most popular methods for integrating the equations of elastodynamics in time, and it enjoys widespread use throughout the field of structural dynamics and other fields such as molecular dynamics.

The HHT- $\alpha$  method is often solved using a predictor-multi-corrector algorithm as well. The full algorithm is summarized in the flow chart on the next page. The only remaining difference between the Newmark method and the HHT- $\alpha$  method is the definition of  $\underline{\underline{M}}^*$ , namely:

$$\underline{\underline{M}}^* = \left\{ \begin{array}{l} \underline{\underline{M}} + \alpha \Delta t \underline{\underline{C}} + \alpha \beta (\Delta t)^2 \underline{\underline{K}} \\ \quad \quad \quad \uparrow \\ \quad \quad \quad \gamma \\ \underline{\underline{M}} \end{array} \right.$$

Consistent  
(converges after one  
step)

Lumped mass approximation

