# Notes on Time Stepping for OOF2

OOF Team

## ZIENKIEWICZ & TAYLOR'S SS22 ALGORITHM

The equation to be solved is

$$\mathbf{M}\ddot{a} + \mathbf{C}\dot{a} + \mathbf{K}a + \mathbf{f} = 0 \tag{1}$$

where $a$ is a vector of values and $\mathbf{M}$, $\mathbf{C}$, and $\mathbf{K}$ are constants.

Assume we know $a$ and $\dot{a}$ at $t = t_n$ and we want to find them at $t = t_{n+1} = t_n + \Delta t$. Expand in a Taylor series in $\tau = t - t_n$:

$$a = a_n + \tau\dot{a}_n + \frac{1}{2}\tau^2\alpha_n \tag{2}$$

$\alpha_n$ is a vector of unknown values. Average (1) over the interval using a weighting function $W(\tau)$:

$$0 = \left[\int_0^{\Delta t} W(\tau)d\tau\right]^{-1} \int_0^{\Delta t} d\tau\, W(\tau)\; [\mathbf{M}\ddot{a} + \mathbf{C}\dot{a} + \mathbf{K}a + \mathbf{f}] \tag{3}$$

Insert (2)

$$0 = \left[\int W(\tau)d\tau\right]^{-1} \int W(\tau) \left(\mathbf{M}\alpha_n + \mathbf{C}(\dot{a}_n + \tau\alpha_n) + \mathbf{K}(a_n + \tau\dot{a}_n + \frac{1}{2}\tau^2\alpha_n) + \mathbf{f}\right) d\tau \tag{4}$$

Since the matrices are constant, we can pull them out of the integral, so if we define

$$\Delta t^k\theta_k = \frac{\int_0^{\Delta t} W(\tau)\tau^k\, d\tau}{\int_0^{\Delta t} W(\tau)\, d\tau} \tag{5}$$

then (4) becomes

$$\begin{aligned} 0 &= \mathbf{M}\alpha_n + \mathbf{C}(\dot{a}_n + \theta_1\Delta t\alpha_n) + \mathbf{K}(a_n + \theta_1\Delta t\dot{a}_n + \frac{1}{2}\Delta t^2\theta_2\alpha_n) + \bar{\mathbf{f}} && (6)\\ &= \left(\mathbf{M} + \theta_1\Delta t\mathbf{C} + \frac{1}{2}\theta_2\Delta t^2\mathbf{K}\right)\alpha_n + (\mathbf{C} + \theta_1\Delta t\mathbf{K})\,\dot{a}_n + \mathbf{K}a_n + \bar{\mathbf{f}} && (7)\end{aligned}$$

where

$$\bar{\mathbf{f}} = \frac{\int_0^{\Delta t} W(\tau)f(t_n+\tau)\, d\tau}{\int_0^{\Delta t} W(\tau)\, d\tau} \tag{8}$$

(7) is a matrix equation which can be solved for $\alpha_n$. Then

$$\begin{aligned} a_{n+1} &= a_n + \Delta t \dot{a}_n + \frac{1}{2}\Delta t^2 \alpha_n && (9) \\ \dot{a}_{n+1} &= \dot{a}_n + \Delta t \alpha_n && (10) \end{aligned}$$

Z&T give no guidance on how to compute $\bar{\mathbf{f}}$ in (7) except to mention that if we assume $\mathbf{f}(t)$ to be linear in $t$ over the (short) interval $\Delta t$ (see below) then

$$\bar{\mathbf{f}} = (1-\theta_1)\mathbf{f}(t_n) + \theta_1 \mathbf{f}(t_{n+1}) \quad (11)$$

which is probably a reasonable approximation.

If $\mathbf{M} = 0$, the equation is a first order ODE in disguise. The method still works as long as we choose the right initial value for $\dot{a}_0$. Just set $\Delta t = 0$ and $\mathbf{M} = 0$ in (7) to get

$$\dot{a}_0 = -\mathbf{C}^{-1}(\mathbf{K}a_0 + \bar{\mathbf{f}}). \quad (12)$$

## NONLINEAR GENERALIZATION OF SS22

If $\mathbf{M}$, $\mathbf{C}$, or $\mathbf{K}$ are functions of the variables $a$ or $t$, we can make progress by assuming that they vary linearly over the interval $\Delta t$, like this:

$$\mathbf{M}(\tau) = \mathbf{M}_n + \frac{\tau}{\Delta t}(\mathbf{M}_{n+1} - \mathbf{M}_n) \quad (13)$$

where $\mathbf{M}_n$ means $\mathbf{M}(t_n, a_n)$. The $\mathbf{M}$ terms in (4) become

$$\left[\int W(\tau) d\tau\right]^{-1} \int W(\tau)\mathbf{M}\alpha_n \, d\tau = (1-\theta_1)\mathbf{M}_n\alpha_n + \theta_1 \mathbf{M}_{n+1}\alpha_n \quad (14)$$

In the linear system, where $\mathbf{M}_n = \mathbf{M}_{n+1} = \mathbf{M}$, this reduces to $\mathbf{M}\alpha_n$, in agreement with (7).

The numerator of the $\mathbf{C}$ terms in (4) becomes

$$\begin{aligned} &\int W(\tau)\mathbf{C}(\dot{a}_n + \tau\alpha_n)\, d\tau \\ &= \int W(\tau)\left(\mathbf{C}_n + \frac{\tau}{\Delta t}(\mathbf{C}_{n+1} - \mathbf{C}_n)\right)(\dot{a}_n + \tau\alpha_n)\, dt && (15) \\ &= \int W(\tau)\left[\mathbf{C}_n\dot{a}_n + \frac{\tau}{\Delta t}(\mathbf{C}_{n+1} - \mathbf{C}_n)\dot{a}_n + \mathbf{C}_n\tau\alpha_n + \frac{\tau^2}{\Delta t}(\mathbf{C}_{n+1} - \mathbf{C}_n)\alpha_n\right] dt && (16) \end{aligned}$$

Use (5) and restore the denominator to get

$$\begin{aligned} &= \mathbf{C}_n\dot{a}_n + \theta_1(\mathbf{C}_{n+1} - \mathbf{C}_n)\dot{a}_n + \Delta t\theta_1\mathbf{C}_n\alpha_n + \Delta t\theta_2(\mathbf{C}_{n+1} - \mathbf{C}_n)\alpha_n && (17) \\ &= \Delta t\left[(\theta_1 - \theta_2)\mathbf{C}_n + \theta_2\mathbf{C}_{n+1}\right]\alpha_n + \left[(1-\theta_1)\mathbf{C}_n + \theta_1\mathbf{C}_{n+1}\right]\dot{a}_n && (18) \end{aligned}$$

In the linear case where $\mathbf{C}_{n+1} = \mathbf{C}_n = \mathbf{C}$, this reduces to $\Delta t\theta_1 \mathbf{C}\alpha_n + \mathbf{C}\dot{a}_n$, also in agreement with (7).

The numerator of the $\mathbf{K}$ terms in (4) becomes

$$\begin{aligned}
&\int W(\tau)\mathbf{K}(a_n + \tau\dot{a}_n + \frac{1}{2}\tau^2\alpha_n) \\
&\quad = \int W(\tau)\left[\mathbf{K}_n + \frac{\tau}{\Delta t}(\mathbf{K}_{n+1} - \mathbf{K}_n)\right](a_n + \tau\dot{a}_n + \frac{1}{2}\tau^2\alpha_n) \qquad (19)
\end{aligned}$$

Including the denominator gives

$$\begin{aligned}
= &\ [(1-\theta_1)\mathbf{K}_n + \theta_1\mathbf{K}_{n+1}]\,a_n + [(\theta_1-\theta_2)\mathbf{K}_n + \theta_2\mathbf{K}_{n+1}]\,\Delta t\dot{a}_n \qquad (20) \\
&+\frac{1}{2}[(\theta_2-\theta_3)\mathbf{K}_n + \theta_3\mathbf{K}_{n+1}]\,\Delta t^2\alpha_n
\end{aligned}$$

When $\mathbf{K}_n = \mathbf{K}_{n+1} = \mathbf{K}$, this reduces to $\mathbf{K}a_n + \theta_1\Delta t\mathbf{K}\dot{a}_n + \frac{1}{2}\theta_2\Delta t^2\mathbf{K}\alpha_n$, in agreement with (7).

Combining (20), (18), and (13), we get

$$0 = \mathbf{M}^*\alpha_n + \mathbf{C}^*\dot{a}_n + \mathbf{K}^*a_n + \bar{\mathbf{f}}^* \qquad (21)$$

where

$$\begin{aligned}
\mathbf{M}^* &= (1-\theta_1)\mathbf{M}_n + \theta_1\mathbf{M}_{n+1} + \Delta t\,[(\theta_1-\theta_2)\mathbf{C}_n + \theta_2\mathbf{C}_{n+1}] \qquad (22) \\
&\quad +\frac{1}{2}\Delta t^2\,[(\theta_2-\theta_3)\mathbf{K}_n + \theta_3\mathbf{K}_{n+1}] \\
\mathbf{C}^* &= (1-\theta_1)\mathbf{C}_n + \theta_1\mathbf{C}_{n+1} + \Delta t\,[(\theta_1-\theta_2)\mathbf{K}_n + \theta_2\mathbf{K}_{n+1}] \qquad (23) \\
\mathbf{K}^* &= (1-\theta_1)\mathbf{K}_n + \theta_1\mathbf{K}_{n+1} \qquad (24) \\
\bar{\mathbf{f}}^* &= (1-\theta_1)\mathbf{f}_n + \theta_1\mathbf{f}_{n+1} \qquad (25)
\end{aligned}$$

(21) is a matrix equation which may be solved for $\alpha_n$, which then determines $a_{n+1}$ and $\dot{a}_{n+1}$ via (9) and (10). Since $\mathbf{M}_{n+1}$, $\mathbf{C}_{n+1}$, $\mathbf{K}_{n+1}$, and $\mathbf{f}_{n+1}$ may depend on $a_{n+1}$, (21) is non-linear and must be solved iteratively, probably with Picard iteration.

It's likely that stability requires that $\theta_i \geq \frac{1}{2}$ for $i = 1, 2, 3$.

## THE NUMERICAL RECIPES METHOD

I'm calling this the Numerical Recipes Method because it's basically the only way that NR suggests handling second order time derivatives. It's not meant to imply that NR invented it. Surprisingly, Z&T *don't* mention this method.

In (1), let

$$y \equiv \mathbf{D}^{-1}\dot{a} \tag{26}$$

where $\mathbf{D}$ is an arbitrary nonsingular matrix. Then we have two *first* order ODEs:

$$\begin{aligned} \mathbf{MD}\dot{y} + \mathbf{CD}y + \mathbf{K}a + \mathbf{f} &= 0 && (27) \\ \dot{a} - \mathbf{D}y &= 0 && (28) \end{aligned}$$

If we define a new vector that includes the degrees of freedom ($a$) and their derivatives ($y$)

$$u = \begin{bmatrix} a \\ y \end{bmatrix} \tag{29}$$

then the equations can be written as

$$\tilde{\mathbf{M}}\dot{u} + \tilde{\mathbf{K}}u + \tilde{f} = 0 \tag{30}$$

where

$$\tilde{\mathbf{M}} = \begin{bmatrix} 0 & \mathbf{MD} \\ \mathcal{I} & 0 \end{bmatrix}, \tag{31}$$

$$\tilde{\mathbf{K}} = \begin{bmatrix} \mathbf{K} & \mathbf{CD} \\ 0 & -\mathbf{D} \end{bmatrix}, \tag{32}$$

and

$$\tilde{f} = \begin{bmatrix} \mathbf{f} \\ 0 \end{bmatrix} \tag{33}$$

If we choose $\mathbf{D} \approx \mathbf{M}^{-1}$, then $\tilde{\mathbf{M}}$ should be well behaved. (30) can be solved with a number of different methods, such as forward and backward Euler, Runge-Kutta, *etc.*