

An analysis of the case where $\theta = 0$

First, we can begin with the derivation of the theta method (TODO: vernacular? this wasn't clear online). This begins with the iterative definition of v , specifically

$$\frac{v^{n+1} - v^n}{\Delta t} = Dv_{zz}^{n+\theta} + \dot{Q}^{n+\theta}$$

Note that if $\theta = 1/2$, this is known as the ‘‘Crank-Nicolson implicit method’’ [1]. Let v_{zz} (using the partial notation such that $v_{zz} = \frac{\partial^2 v}{\partial z^2}$) be defined as

$$v_{zz}^{n+\theta} := \theta v_{zz}^{n+1} + (1 - \theta)v_{zz}^n$$

Then Q can be defined by the relationship

$$\tau \frac{Q^{n+1} - Q^n}{\Delta t} + Q^n = \epsilon v_{zz}^n$$

And then reformulated for Q^{n+1} as

$$Q^{n+1} = Q^n - \frac{\Delta t}{\tau} Q^n + \frac{\epsilon \Delta t}{\tau} v_{zz}^n$$

Note that this segment of code is where polynomial chaos will shortly be implemented. Now that the $n + 1$ th value of Q has been found, a simple finite difference can be utilized in order to find its time derivative:

$$\dot{Q}^{n+1/2} = \frac{Q^{n+1} - Q^n}{\Delta t}$$

Finally, this new data can be utilized to solve for the $n + 1$ th value of v , specifically in the form of

$$v^{n+1} = v^n + \theta D \Delta t A v^{n+1} + (1 - \theta) D \Delta t A v^n + \Delta t \dot{Q}^{n+1/2}$$

However this is not in its final form, and can be simplified slightly further in order to reach usability:

$$v^{n+1} = (I - \theta D \Delta t A)^{-1} \left[v^n + (1 - \theta) D \Delta t A v^n + \Delta t \dot{Q}^{n+1/2} \right]$$

We can then analyze the special case where $\theta = 0$. In this instance, v^{n+1} can be written as (using the fact that the identity matrix is its own inverse)

$$v^{n+1} = \left[v^n + D \Delta t A v^n + \Delta t \dot{Q}^{n+1/2} \right]$$

Which is the same as the case in which the theta method is not implemented, with the definition $D = \kappa H_A G_\infty$ (TODO: is this the same?):

$$v^{n+1} = v^n + \Delta t D v_{zz}^n + \Delta t \kappa H_A \dot{Q}^{n+1/2}$$

0.1 Advantage of using Crank-Nicolson

In the case where $\theta = 0$, the Courant-Friedrichs-Lewy condition (CFL condition) applies as a necessary condition for convergence (due to the fact that we are solving partial differential equations numerically by finite differences), specifically following a second order nonlinear finite difference, of the form

$$\frac{\Delta t}{(\Delta x)^2} < C_u$$

When time steps larger than this calculated value are utilized, the output results become unstable:

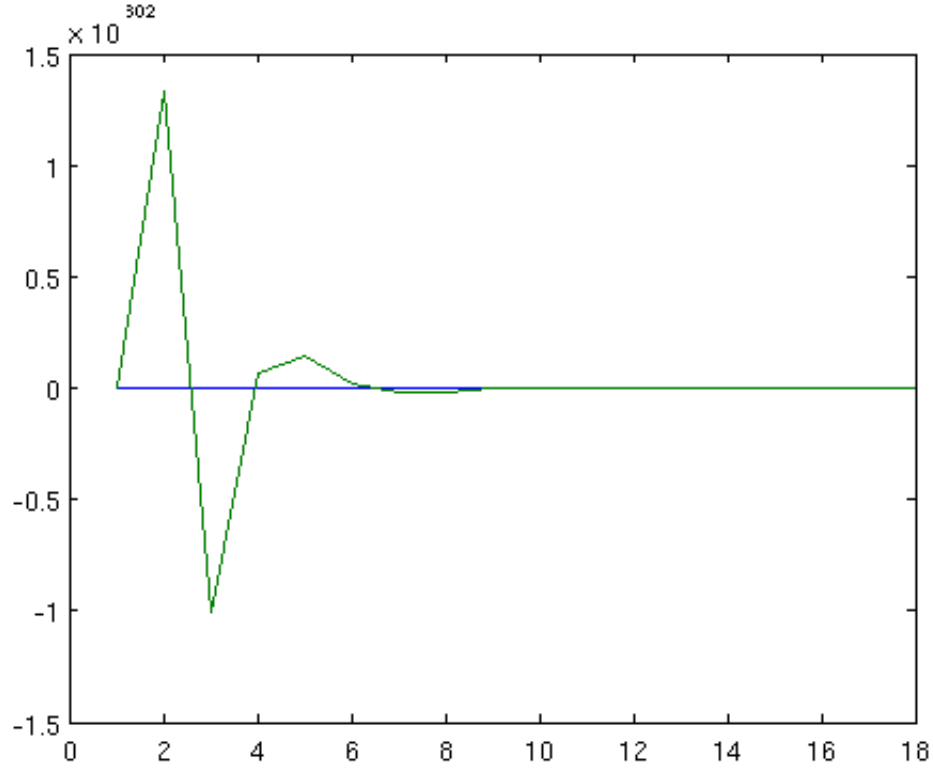


Figure 1: An example of usage of an overly large time step Δt

Which, in this specific case, Δt becomes

$$\Delta t = \frac{(\Delta z)^2}{2\kappa H_A G_\infty}$$

Furthermore, a safety factor^[citation needed] is commonly used in order to ensure stability of the time step. When set to 0.9, this is called the Mingham safety factor^[citation needed]

References

- [1] Crank, J., Nicolson, P.: A practical method for numerical evaluation of solutions of partial differential equations of the heat conduction type. Proceedings of the Cambridge Philosophical Society 43, 5064 (1947)