Numerical Integration in Time

Vladislav A. Yastrebov

MINES Paris - PSL, CNRS
Centre des Matériaux, Evry, France

Semaine PSL @ Mines Paris
November 27, 2024

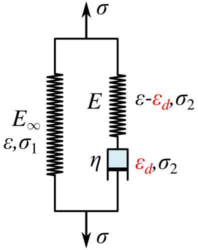
Outline

Motivation

- In nonlinear materials, first order differential equations govern the change of history variables. For example, in viscoelastic material model

$$\sigma = (E + E_\infty)\varepsilon + E\varepsilon_d, \quad \boxed{\dot\varepsilon_d + \frac{\varepsilon_d}{\tau} = \frac{\varepsilon}{\tau}}, \quad \tau = \eta/E$$

with Young's moduli E, E_∞ (Pa), total ε and viscous ε_d strain, viscosity η (Pa·s), relaxation time τ (s).



©Formula 1

Motivation

- In nonlinear materials, first order differential equations govern the change of history variables. For example, in viscoelastic material model

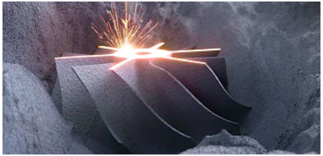
$$\sigma = (E + E_\infty)\varepsilon + E\varepsilon_d, \quad \boxed{\dot\varepsilon_d + \frac{\varepsilon_d}{\tau} = \frac{\varepsilon}{\tau}}, \quad \tau = \eta/E$$

with Young's moduli E, E_∞ (Pa), total ε and viscous ε_d strain, viscosity η (Pa·s), relaxation time τ (s).

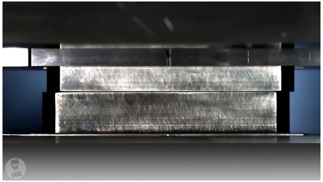
- In non-stationary processes governed by parabolic equations. For example, heat equation

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) \quad \Leftrightarrow \quad \boxed{\dot T = \alpha \Delta T}$$

ρ - density, c_p specific heat capacity at constant pressure, k thermal conductivity.



Additive manufacturing, ©DMG MORI



Friction welding

Motivation

- In solid dynamics, hyperbolic PDE:

$$\boxed{\nabla \cdot \underline{\underline{\sigma}} + \underline{f} = \rho \underline{\ddot{u}}}$$

Lego-car crash simumation in LS-DYNA, ©DYNAMORE

Variable separation

- Search solution in time:

$$\{\underline{\boldsymbol{X}}, t\} \in \Omega \times (0, T] :\rightarrow \underline{\boldsymbol{u}}(\underline{\boldsymbol{X}}, t)$$

- Variable separation:

$$\underline{\boldsymbol{u}}(\underline{\boldsymbol{X}}, t) = \sum N_i(\underline{\boldsymbol{X}})\underline{\boldsymbol{u}}_i(t)$$

Variable separation

- Search solution in time:

$$\{\underline{X}, t\} \in \Omega \times (0, T] :\to \underline{u}(\underline{X}, t)$$

- Variable separation:

$$\underline{u}(\underline{X}, t) = \sum N_i(\underline{X})\underline{u}_i(t)$$

- Results in 2nd order in time system of ODE:

$$[M][\ddot{u}] + [C][\dot{u}] + [K][u] = [F](t)$$

with mass matrix $[M] \in \mathbb{R}^{n\times n}$,
viscous damping matrix $[C] \in \mathbb{R}^{n\times n}$,
stiffness matrix $[K] \in \mathbb{R}^{n\times n}$,
unknown displacements $[u] \in \mathbb{R}^{n}$.

Variable separation

- Search solution in time:

$$\{\underline{X}, t\} \in \Omega \times (0, T] :\to \underline{u}(\underline{X}, t)$$

- Variable separation:

$$\underline{u}(\underline{X}, t) = \sum N_i(\underline{X})\underline{u}_i(t)$$

- Results in 2nd order in time system of ODE:

$$[M][\ddot{u}] + [C][\dot{u}] + [K][u] = [F](t)$$

with mass matrix $[M] \in \mathbb{R}^{n\times n}$,
viscous damping matrix $[C] \in \mathbb{R}^{n\times n}$,
stiffness matrix $[K] \in \mathbb{R}^{n\times n}$,
unknown displacements $[u] \in \mathbb{R}^{n}$.

- Or in 1st order in time system of ODE:

$$[C][\dot{T}] + [K][T] = [Q](t)$$

First order differential equations

First order ODE

- Consider a linear first order system of ODE

$$[\dot{q}] = f([q]; t)$$

First order ODE

- Consider a linear first order system of ODE

$$[\dot{q}] = f([q]; t), \quad t \in \mathcal{T} = [0, T] \subset \mathbb{R}, \quad [q] \in \mathbb{R}^n$$

First order ODE

- Consider a linear first order system of ODE

$$[\dot{q}] = f([q]; t), \quad t \in \mathcal{T} = [0, T] \subset \mathbb{R}, \quad [q] \in \mathbb{R}^n$$

- With initial conditions:

$$[q](t = 0) = [q_0]$$

we get a Cauchy problem.

First order ODE

- Consider a linear first order system of ODE

$$[\dot{q}] = f([q];t), \quad t \in \mathcal{T} = [0,T] \subset \mathbb{R}, \quad [q] \in \mathbb{R}^n$$

- With initial conditions:

$$[q](t=0) = [q_0]$$

  we get a Cauchy problem.
- Cauchy-Lipschitz (or Picard–Lindelöf) theorem:

  (1) If function $f : \mathbb{R}^n \times \mathcal{T} \to \mathbb{R}^n$ *is continuous in* t*:* $f(\bullet, t) \in C^0(\mathcal{T})$

First order ODE

- Consider a linear first order system of ODE

$$[\dot q] = f([q];t), \quad t \in \mathcal{T} = [0,T] \subset \mathbb{R}, \quad [q] \in \mathbb{R}^n$$

- With initial conditions:

$$[q](t=0) = [q_0]$$

  we get a Cauchy problem.

- Cauchy-Lipschitz (or Picard–Lindelöf) theorem:

  (1) If function $f : \mathbb{R}^n \times \mathcal{T} \to \mathbb{R}^n$ is continuous in t: $f(\bullet, t) \in C^0(\mathcal{T})$

  (2) and is Lipschitz continuous in $[q]$,

First order ODE

- Consider a linear first order system of ODE

$$[\dot q] = f([q];t), \quad t \in \mathcal{T} = [0,T] \subset \mathbb{R}, \quad [q] \in \mathbb{R}^n$$

- With initial conditions:

$$[q](t=0) = [q_0]$$

  we get a Cauchy problem.
- Cauchy-Lipschitz (or Picard–Lindelöf) theorem:
  (1) If function $f : \mathbb{R}^n \times \mathcal{T} \to \mathbb{R}^n$ is continuous in t: $f(\bullet,t) \in C^0(\mathcal{T})$
  (2) and is Lipschitz continuous in $[q]$,

$$\exists K \geq 0 \; s.t. \; \forall t \in \mathcal{T}, \forall [q],[q]' \in \mathbb{R}^n : \left\| f([q];t) - f([q]';t) \right\| \leq K \left\| [q] - [q]' \right\|,$$

First order ODE

- Consider a linear first order system of ODE

$$[\dot{q}] = f([q];t), \quad t \in \mathcal{T} = [0,T] \subset \mathbb{R}, \quad [q] \in \mathbb{R}^n$$

- With initial conditions:

$$[q](t=0) = [q_0]$$

we get a Cauchy problem.

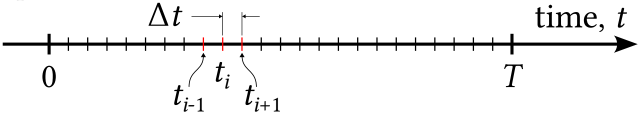
- Cauchy-Lipschitz (or Picard–Lindelöf) theorem:

  (1) If function $f : \mathbb{R}^n \times \mathcal{T} \to \mathbb{R}^n$ is continuous in t: $f(\bullet, t) \in C^0(\mathcal{T})$
  (2) and is Lipschitz continuous in $[q]$,

$$\exists K \geq 0 \; s.t. \; \forall t \in \mathcal{T}, \forall [q],[q]' \in \mathbb{R}^n : \left\| f([q];t) - f([q]';t) \right\| \leq K \left\| [q] - [q]' \right\|,$$

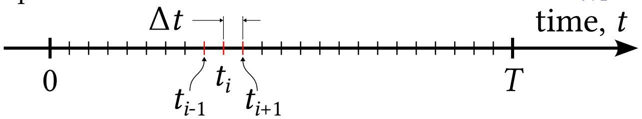
  then $\forall [q_0] \in \mathbb{R}^n$, a unique solution $[q(t)]$ for Cauchy problem exists.

- Split time interval into uniform increments $\Delta t = t_{i+1} - t_i$



Discretization

- Split time interval into uniform increments $\Delta t = t_{i+1} - t_i$



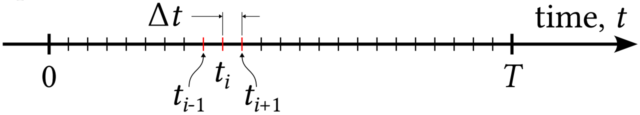
- Taylor expansion:

$$[\boldsymbol{q}(\boldsymbol{t} + \boldsymbol{\Delta t})] = [\boldsymbol{q}(\boldsymbol{t})] + [\dot{\boldsymbol{q}}(\boldsymbol{t})]\Delta t + \frac{1}{2}[\ddot{\boldsymbol{q}}(\boldsymbol{t})]\Delta t^2 + o(\Delta t^2)$$

with Bachmann-Landau or asymptotic notations: $y = o(x)$ if $y/x \xrightarrow{x\to 0} 0$

Discretization

- Split time interval into uniform increments $\Delta t = t_{i+1} - t_i$



- Taylor expansion:

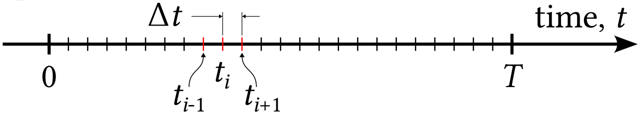
$$[q(t + \Delta t)] = [q(t)] + [\dot{q}(t)]\Delta t + \frac{1}{2}[\ddot{q}(t)]\Delta t^2 + o(\Delta t^2)$$

with Bachmann-Landau or asymptotic notations: $y = o(x)$ if $y/x \xrightarrow{x\to 0} 0$

- So we search discrete values: $[q]_k = [q(t_k)]$

Discretization

- Split time interval into uniform increments $\Delta t = t_{i+1} - t_i$



- Taylor expansion:

$$[q(t+\Delta t)] = [q(t)] + [\dot q(t)]\Delta t + \frac{1}{2}[\ddot q(t)]\Delta t^2 + o(\Delta t^2)$$

  with Bachmann-Landau or asymptotic notations: $y = o(x)$ if $y/x \xrightarrow{x\to 0} 0$

- So we search discrete values: $[q]_k = [q(t_k)]$
- An integration method is consistent iff

$$\lim_{\Delta t\to 0} \frac{[q]_{k+1} - [q]_k}{\Delta t} = [\dot q(t_k)]$$

Integration in time

- We know that

$$[q]_{k+1} = [q]_k + \int\limits_{t_k}^{t_k+1} [\dot{q}]dt$$

Integration in time

- We know that

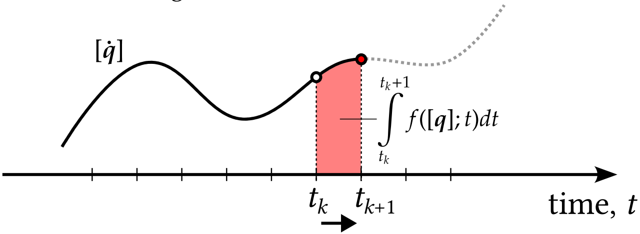
$$[\boldsymbol{q}]_{k+1} = [\boldsymbol{q}]_k + \int\limits_{t_k}^{t_k+1} [\dot{\boldsymbol{q}}]dt = [\boldsymbol{q}]_k + \int\limits_{t_k}^{t_k+1} f([\boldsymbol{q}];t)dt$$

Integration in time

- We know that

$$[q]_{k+1} = [q]_k + \int\limits_{t_k}^{t_k+1} [\dot q]dt = [q]_k + \int\limits_{t_k}^{t_k+1} f([q];t)dt$$

- Why not to use known integration methods?

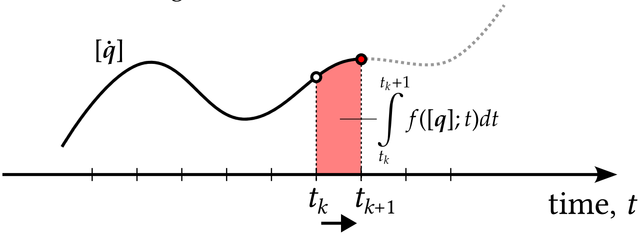


Integration in time

- We know that

$$[q]_{k+1} = [q]_k + \int\limits_{t_k}^{t_k+1} [\dot{q}]dt = [q]_k + \int\limits_{t_k}^{t_k+1} f([q];t)dt$$

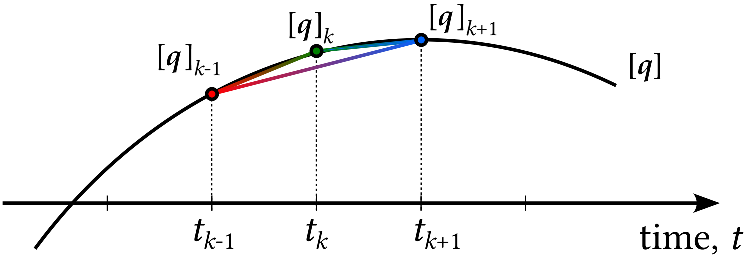
- Why not to use known integration methods?



- Because the value of the integrand in unknown

$$\int\limits_{t_k}^{t_k+1} f([q];t)dt = ?$$

Finite difference



Finite difference

- Consider left and right Taylor expansions:

$$[\boldsymbol{q}(\boldsymbol{t}_k + \boldsymbol{\Delta t})] = [q]_{k+1} = [q]_k + [\dot{q}]_k \Delta t + \frac{1}{2}[\ddot{q}]_k \Delta t^2 + o(\Delta t^2)$$

$$[\boldsymbol{q}(\boldsymbol{t}_k - \boldsymbol{\Delta t})] = [q]_{k-1} = [q]_k - [\dot{q}]_k \Delta t + \frac{1}{2}[\ddot{q}]_k \Delta t^2 - o(\Delta t^2)$$

Finite difference

- Consider left and right Taylor expansions:

$$[\boldsymbol{q(t_k + \Delta t)}] = [q]_{k+1} = [q]_k + [\dot q]_k \Delta t + \frac{1}{2}[\ddot q]_k \Delta t^2 + o(\Delta t^2)$$

$$[\boldsymbol{q(t_k - \Delta t)}] = [q]_{k-1} = [q]_k - [\dot q]_k \Delta t + \frac{1}{2}[\ddot q]_k \Delta t^2 - o(\Delta t^2)$$

- The finite differences are then:

$$[\dot q]_k^h = \frac{[q]_{k+1} - [q]_k}{\Delta t} = [\dot q]_k + \frac{1}{2}[\ddot q]_k \Delta t + o(\Delta t)$$

$$[\dot q]_k^{-h} = \frac{[q]_k - [q]_{k-1}}{\Delta t} = [\dot q]_k - \frac{1}{2}[\ddot q]_k \Delta t + o(\Delta t)$$

- And the central difference:

$$[\dot q]_k^{\circ h} = \frac{[q]_{k+1} - [q]_{k-1}}{2\Delta t} = [\dot q]_k + o(\Delta t)$$

Finite difference II

- In first order approximation:

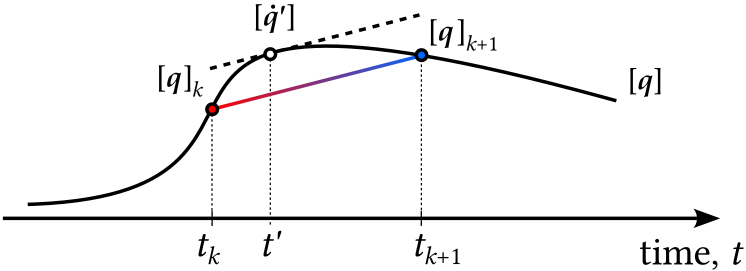
$$[\dot{q}]_k = \frac{[q]_{k+1} - [q]_k}{\Delta t} + O(\Delta t)$$

$$[\dot{q}]_k = \frac{[q]_k - [q]_{k-1}}{\Delta t} + O(\Delta t)$$

$$[\dot{q}]_k = \frac{[q]_{k+1} - [q]_{k-1}}{2\Delta t} + O(\Delta t^2)$$

- Note that notation $o(\Delta t)$ was changed to $O(\Delta t)$, where $y = O(x)$ means that $0 < \lim\limits_{x\to 0} |y/x| < \infty$.

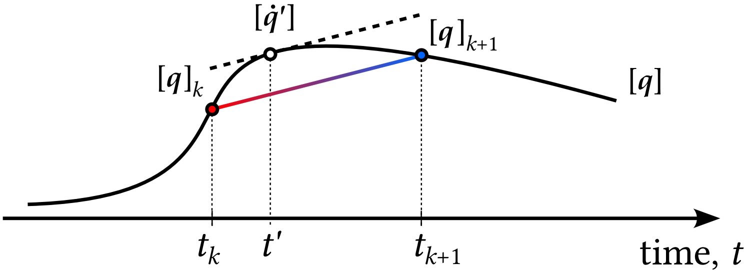
Mean value theorem



Th: If $[q] \in C^1([t_k, t_{k+1}])$ then $\exists t' \in [t_k, t_{k+1}]$ such that

$$[q]_{k+1} - [q]_k = [\dot q(t')](t_{k+1} - t_k)$$

Mean value theorem



Th: If $[q] \in C^1([t_k, t_{k+1}])$ then $\exists t' \in [t_k, t_{k+1}]$ such that

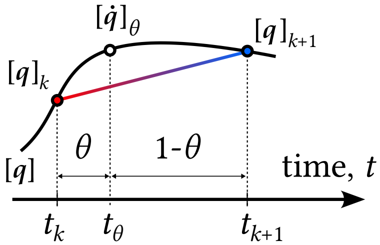
$$[q]_{k+1} - [q]_k = [\dot{q}(t')](t_{k+1} - t_k) \quad \Leftrightarrow \quad \frac{[q]_{k+1} - [q]_k}{\Delta t} = [\dot{q}(t')]$$

NB: Théorème des accroissements finis, Théorème de Lagrange

Integration methods

- First order ODE:

$$[\dot q] = f([q];t), \quad t \in \mathcal{T} = [0,T] \subset \mathbb{R}, \quad [q] \in \mathbb{R}^n$$



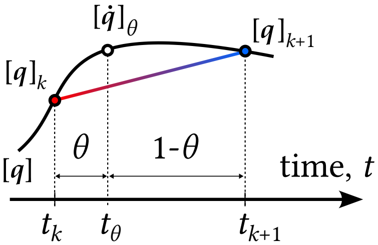
Integration methods

- First order ODE:

$$[\dot q] = f([q];t), \quad t \in \mathcal{T} = [0,T] \subset \mathbb{R}, \quad [q] \in \mathbb{R}^n$$

- Time points:

$$t_k,\ t_{k+1}: \quad \Rightarrow \quad t_\theta = (1-\theta)t_k + \theta t_{k+1} = t_k + \theta \Delta t$$



Integration methods

- First order ODE:

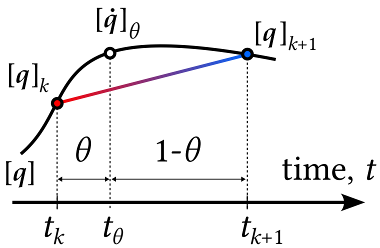
$$[\dot q] = f([q];t), \quad t \in \mathcal{T} = [0,T] \subset \mathbb{R}, \quad [q] \in \mathbb{R}^n$$

- Time points:

$$t_k,\ t_{k+1}: \quad \Rightarrow \quad t_\theta = (1-\theta)t_k + \theta t_{k+1} = t_k + \theta\Delta t$$

- Approximation:

$$\frac{[q]_{k+1} - [q]_k}{\Delta t} \approx f([\boldsymbol{q}(\boldsymbol{t_\theta})]; t_\theta)$$



Integration methods

- First order ODE:

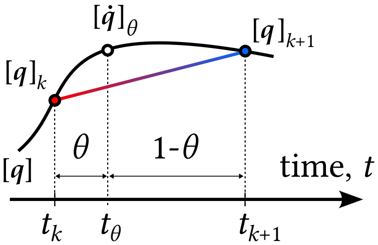
$$[\dot q] = f([q];t), \quad t \in \mathcal{T} = [0,T] \subset \mathbb{R}, \quad [q] \in \mathbb{R}^n$$

- Time points:

$$t_k,\ t_{k+1}: \quad \Rightarrow \quad t_\theta = (1-\theta)t_k + \theta t_{k+1} = t_k + \theta\Delta t$$

- Approximation:

$$\frac{[q]_{k+1} - [q]_k}{\Delta t} \approx f([\boldsymbol{q}(\boldsymbol{t_\theta})]; t_\theta)$$

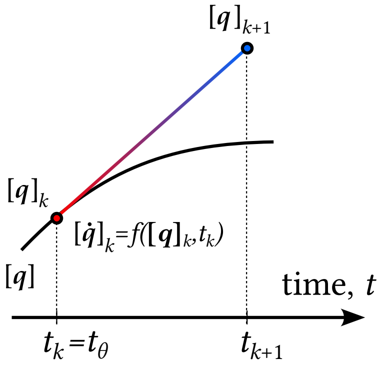


Methods:

- $\theta = 0$: Explicit (forward) Euler
- $\theta = 1$: Implicit (backward) Euler
- ★ $\theta = 0.5$: Crank-Nicolson method

Explicit integration

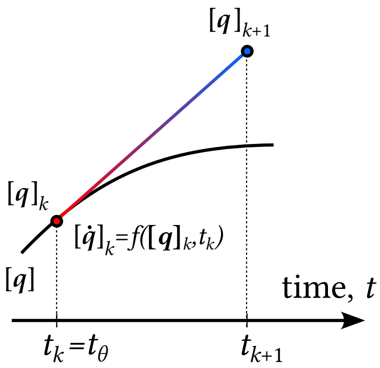
- Since $\theta = 0$, the derivative is found at $t_\theta = t_k$



Explicit integration

- Since $\theta = 0$, the derivative is found at $t_\theta = t_k$
- Approximation:

$$\frac{[q]_{k+1} - [q]_k}{\Delta t} = f([\mathbf{q}(\mathbf{t}_k)]; t_k) + O(\Delta t)$$



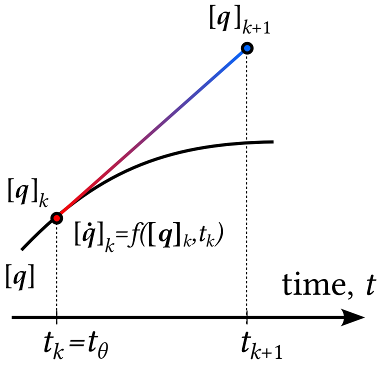
Explicit integration

- Since $\theta = 0$, the derivative is found at $t_\theta = t_k$
- Approximation:

$$\frac{[q]_{k+1} - [q]_k}{\Delta t} = f([\boldsymbol{q}(\boldsymbol{t}_k)]; t_k) + O(\Delta t)$$

- Prediction:

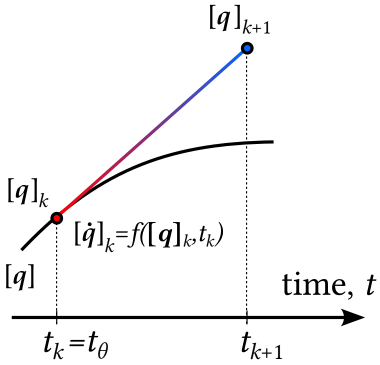
$$[q]_{k+1} = [q]_k + \Delta t\, f([\boldsymbol{q}(\boldsymbol{t}_k)]; t_k) + o(\Delta t)$$



Explicit integration for system of equations

- For system of equations:

$$[C][\dot{q}] + [K][q] = [F(t)]$$



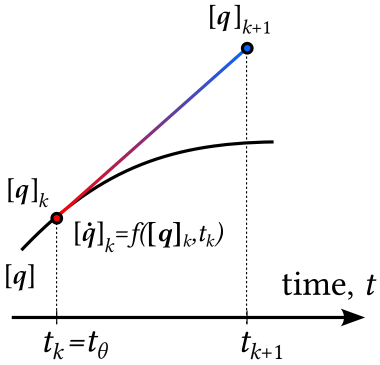
Explicit integration for system of equations

- For system of equations:

$$[C][\dot{q}] + [K][q] = [F(t)]$$

- Canonical form:

$$[\dot{q}] = [C]^{-1}\left([F(t)] - [K][q]\right)$$



Explicit integration for system of equations

- For system of equations:

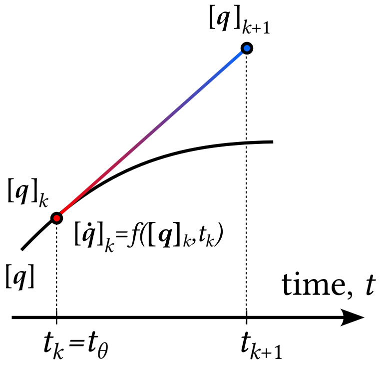
$$[C][\dot q] + [K][q] = [F(t)]$$

- Canonical form:

$$[\dot q] = [C]^{-1}\left([F(t)] - [K][q]\right)$$

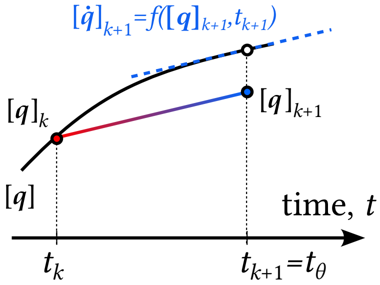
- If $[C]$ is diagonal $[C] = \mathrm{diag}\{c^1, c^2, \cdots, c^n\}$, then using explicit integration

$$q^i_{k+1} = q^i_k + \frac{\Delta t}{c^i}\left([F(t_k)] - [K][q]_k\right)^i$$



Implicit integration

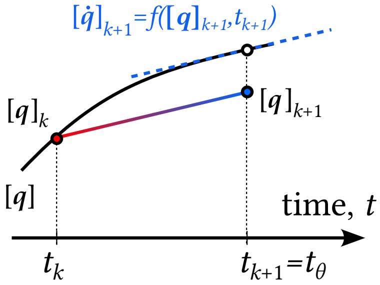
- Since $\theta = 1$, the derivative is found at $t_\theta = t_{k+1}$



Implicit integration

- Since $\theta = 1$, the derivative is found at $t_\theta = t_{k+1}$
- Approximation:

$$\frac{[q]_{k+1} - [q]_k}{\Delta t} = f([q]_{k+1}; t_{k+1}) + O(\Delta t)$$



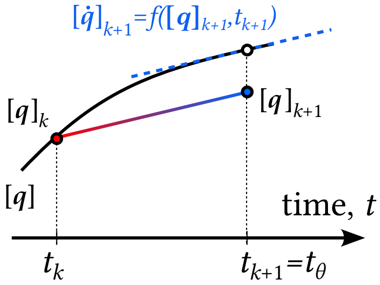
Implicit integration

- Since $\theta = 1$, the derivative is found at $t_\theta = t_{k+1}$
- Approximation:

$$\frac{[q]_{k+1} - [q]_k}{\Delta t} = f([q]_{k+1}; t_{k+1}) + O(\Delta t)$$

- Prediction:

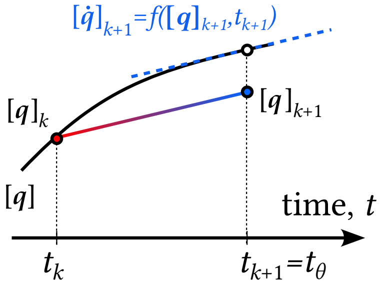
$$[q]_{k+1} = [q]_k + \Delta t\, f([q]_{k+1}; t_{k+1}) + o(\Delta t)$$



Implicit integration for system of equations

- For system of equations:

$$[C][\dot{q}] + [K][q] = [F(t)]$$



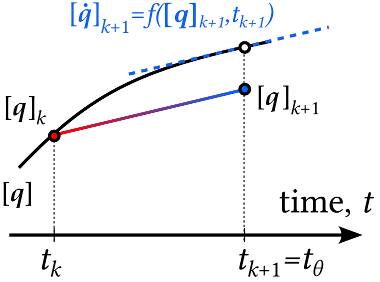
Implicit integration for system of equations

- For system of equations:

$$[C][\dot q] + [K][q] = [F(t)]$$

- Finite difference:

$$[C]\,\big([q]_{k+1} - [q]_k\big) = \Delta t\,\big([F(t_{k+1})] - [K][q]_{k+1}\big) + o(\Delta t)$$



Implicit integration for system of equations

- For system of equations:

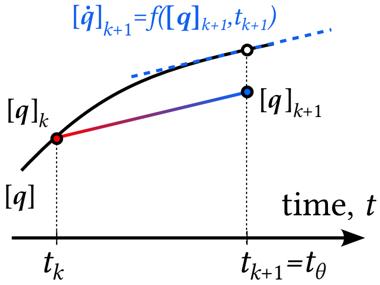
$$[C][\dot{q}] + [K][q] = [F(t)]$$

- Finite difference:

$$[C]\left([q]_{k+1} - [q]_k\right) = \Delta t\left([F(t_{k+1})] - [K][q]_{k+1}\right) + o(\Delta t)$$

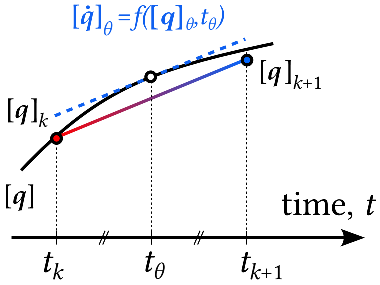
- Linear system of equations to be solved:

$$\Big([C] + \Delta t[K]\Big)[q]_{k+1} = [C][q]_k + \Delta t\,[F(t_{k+1})]$$



Crank-Nicolson integration

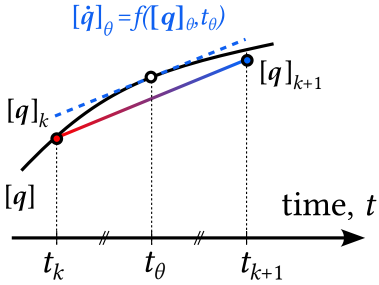
- Since $\theta = 0.5$, the derivative is found at $t_\theta = t_k + 0.5\Delta t = t_{k+1/2}$



Crank-Nicolson integration

- Since $\theta = 0.5$, the derivative is found at $t_\theta = t_k + 0.5\Delta t = t_{k+1/2}$
- Approximation:

$$\frac{[q]_{k+1} - [q]_k}{\Delta t} = f([\mathbf{q}]_{k+1/2}; t_{k+1/2}) + O(\Delta t^2)$$



Crank-Nicolson integration

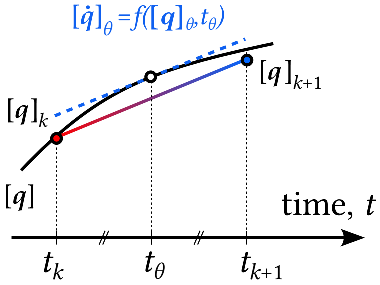
- Since $\theta = 0.5$, the derivative is found at $t_\theta = t_k + 0.5\Delta t = t_{k+1/2}$
- Approximation:

$$\frac{[q]_{k+1} - [q]_k}{\Delta t} = f([q]_{k+1/2}; t_{k+1/2}) + O(\Delta t^2)$$

- Prediction:

$$[q]_{k+1} = [q]_k + \Delta t\, f([q]_{k+1/2}; t_{k+1/2}) + o(\Delta t^2)$$

$$f([q]_{k+1/2}; t_{k+1/2}) \approx \frac{1}{2}\Big(f([q]_{k+1}; t_{k+1}) + f([q]_k; t_k)\Big)$$



Crank-Nicolson integration

- Since $\theta = 0.5$, the derivative is found at $t_\theta = t_k + 0.5\Delta t = t_{k+1/2}$
- Approximation:

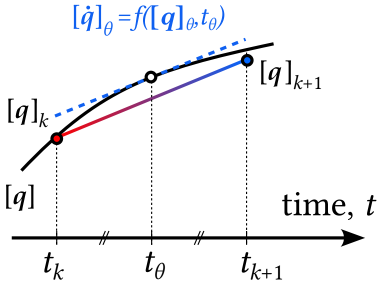
$$\frac{[q]_{k+1} - [q]_k}{\Delta t} = f([q]_{k+1/2}; t_{k+1/2}) + O(\Delta t^2)$$

- Prediction:

$$[q]_{k+1} = [q]_k + \Delta t\, f([q]_{k+1/2}; t_{k+1/2}) + o(\Delta t^2)$$

$$f([q]_{k+1/2}; t_{k+1/2}) \approx \frac{1}{2}\Big(f([q]_{k+1}; t_{k+1}) + f([q]_k; t_k)\Big)$$

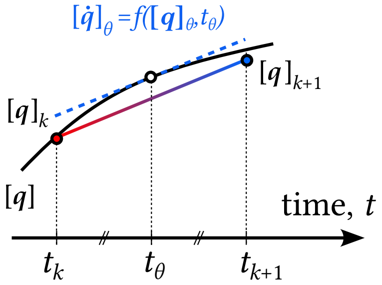
- Finally: $[q]_{k+1} = [q]_k + \frac{\Delta t}{2}\Big(f([q]_{k+1}; t_{k+1}) + f([q]_k; t_k)\Big) + o(\Delta t^2)$



Crank-Nicolson integration for system of equations

- For system of equations:

$$[C][\dot q] + [K][q] = [F(t)]$$



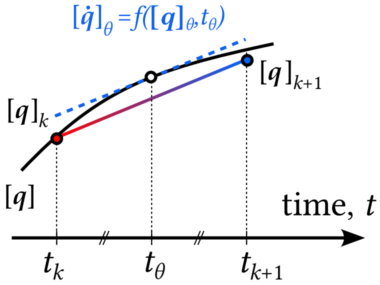
Crank-Nicolson integration for system of equations

- For system of equations:

$$[C][\dot q] + [K][q] = [F(t)]$$

- Finite difference:

$$[C]\left([q]_{k+1} - [q]_k\right) = \frac{\Delta t}{2}\Big([F]_{k+1} + [F]_k - [K]\left([q]_{k+1} + [q]_k\right)\Big) + o(\Delta t^2)$$



Crank-Nicolson integration for system of equations

- For system of equations:

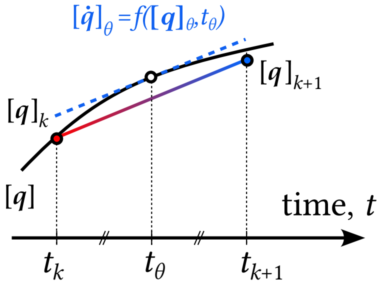
$$[C][\dot q] + [K][q] = [F(t)]$$

- Finite difference:

$$[C]\left([q]_{k+1} - [q]_k\right) = \frac{\Delta t}{2}\Big([F]_{k+1} + [F]_k - [K]\left([q]_{k+1} + [q]_k\right)\Big) + o(\Delta t^2)$$

- Linear system of equations to be solved:

$$\left([C] + \frac{\Delta t}{2}[K]\right)[q]_{k+1} = \left([C] - \frac{\Delta t}{2}[K]\right)[q]_k + \frac{\Delta t}{2}\left([F]_k + [F]_{k+1}\right)$$



Example: 1D heat equation

- PDE

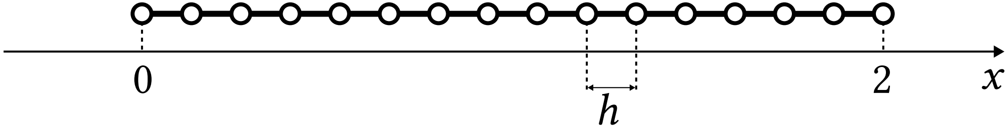
$$\dot{T}(x,t) = \alpha \Delta T(x,t), \quad x \in [0,2], \quad t \in [0,\infty)$$

- Initial conditions

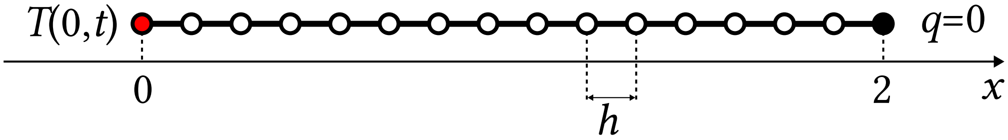
$$T(x,0) = 0$$

- Boundary conditions:
  - Left edge $x = 0$: increase temperature $T(0,t) = T_0 t / t_0$
  - Right edge $x = 2$: zero flux $q = \frac{\partial T}{\partial x}\Big|_{(2,t)} = 0$
- Mesh: $N_x = 40$, $h = 0.05$ (l.u.)
- Parameter: $\alpha = 0.01$ (l.u.^{2}/t.u.)

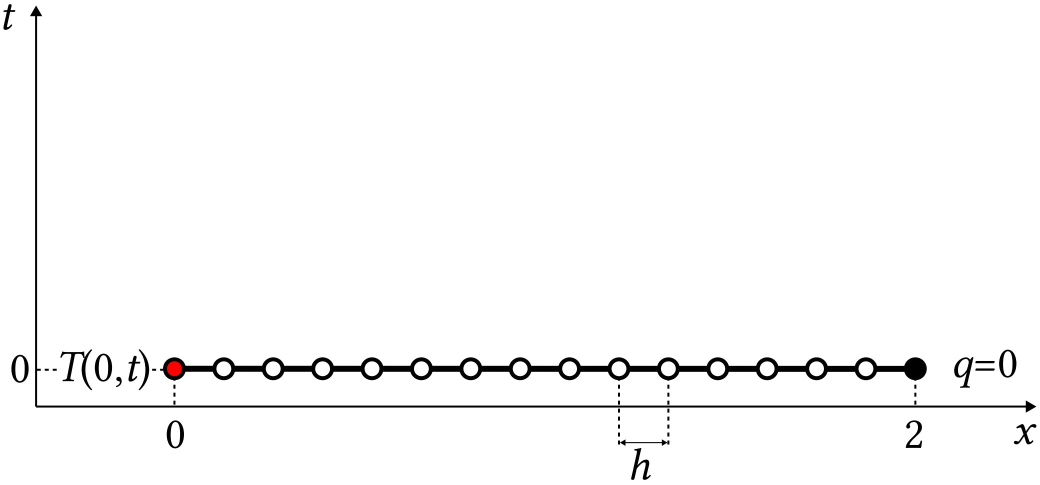
Example: 1D heat equation



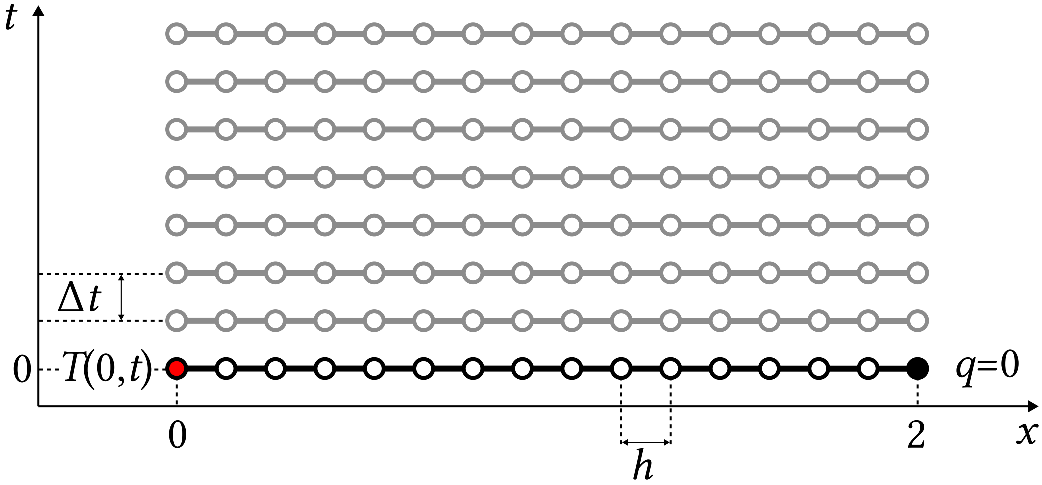
Example: 1D heat equation



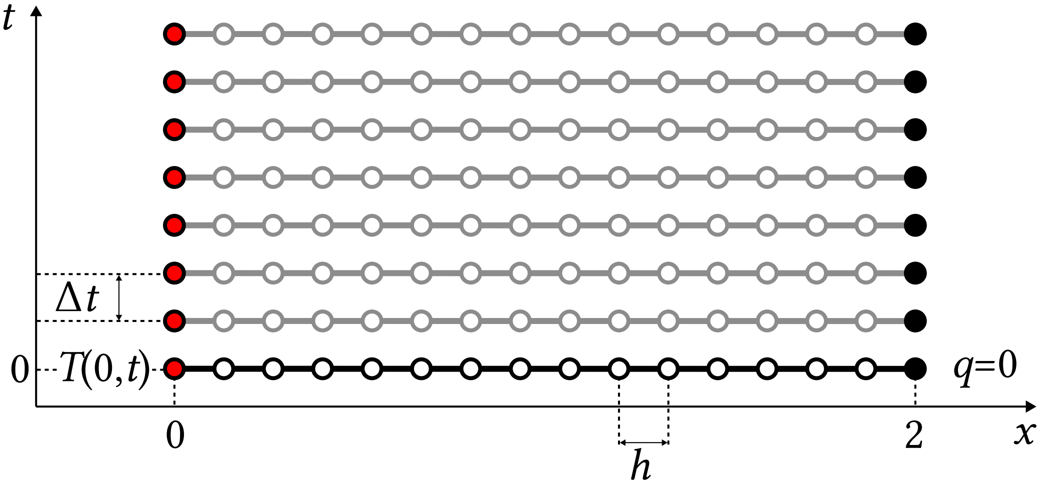
Example: 1D heat equation



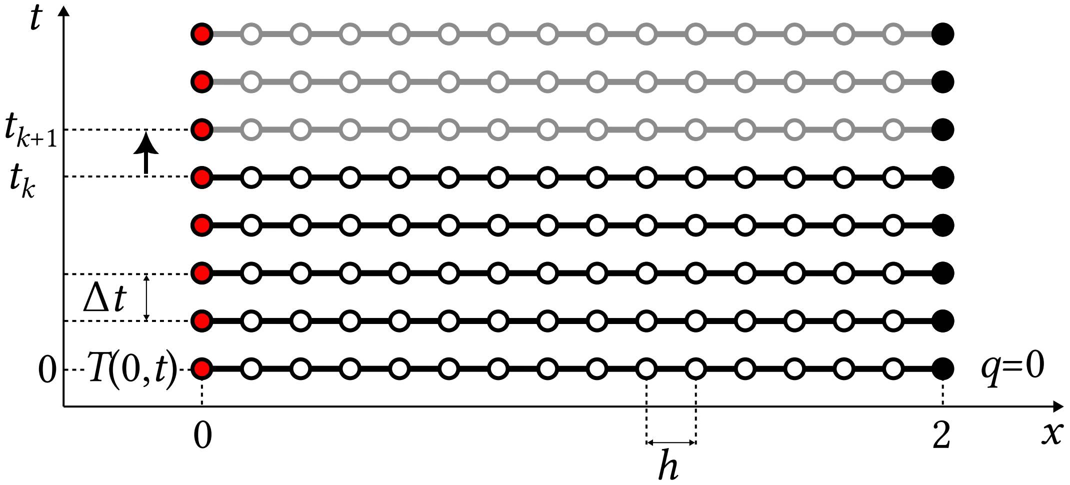
Example: 1D heat equation



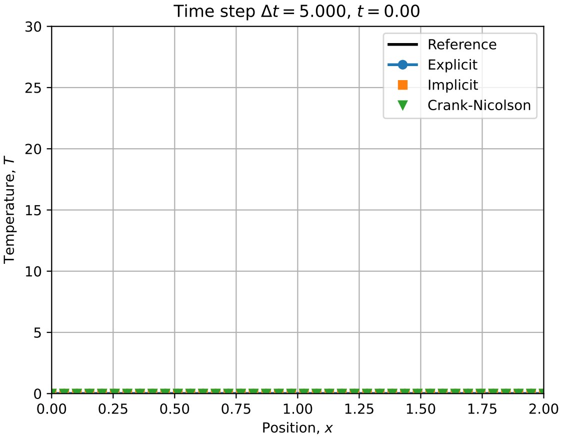
Example: 1D heat equation



Example: 1D heat equation

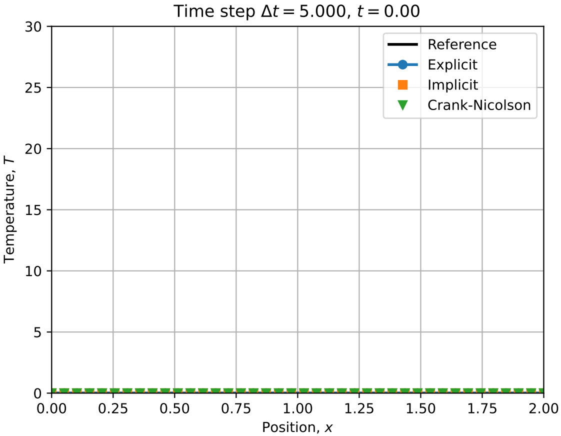


Example: integration results



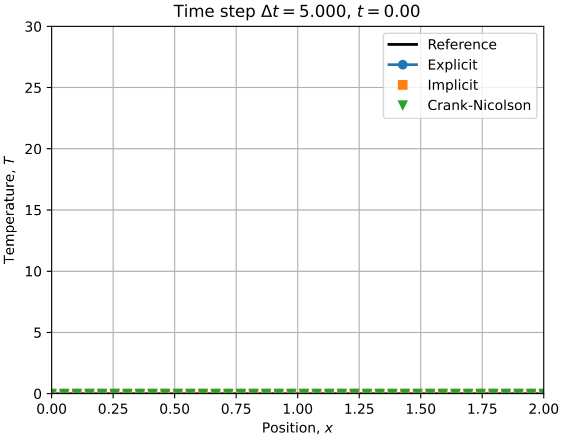
$\Delta t = 0.10$ t.u.

Example: integration results



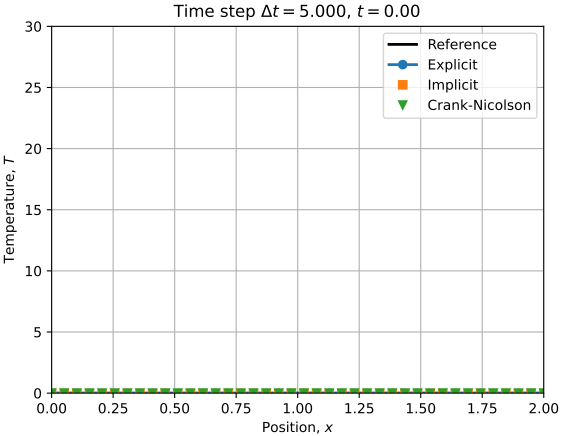
$\Delta t = 0.13$ t.u.

Example: integration results



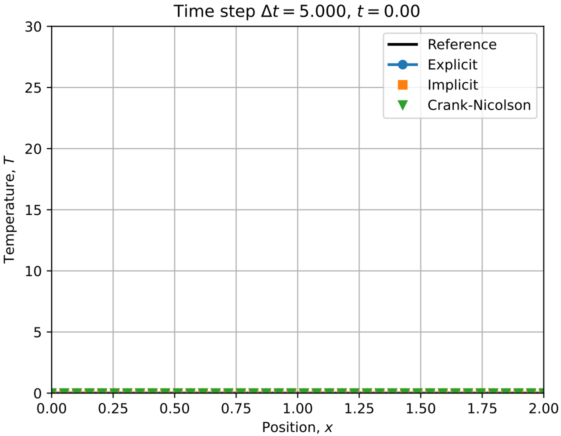
$\Delta t = 1.00$ t.u.

Example: integration results



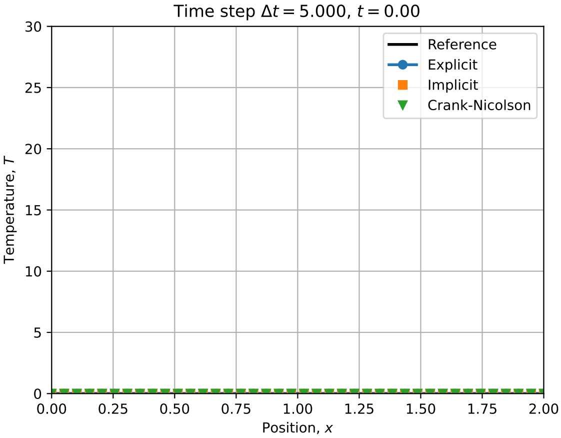
$\Delta t = 2.00$ t.u.

Example: integration results



$\Delta t = 5.00$ t.u.

Example: integration results



$\Delta t = 10.00$ t.u.

Stability criterion

- For $\theta \geq 1/2$ the integration is unconditionally stable

[1] Courant, R.; Friedrichs, K.; Lewy, H. (1928), Über die partiellen Differenzengleichungen der mathematischen Physik (in German), Mathematische Annalen 100 (1): 32-74
[2] Courant, R., Friedrichs, K. and Lewy, H., 1967. On the partial difference equations of mathematical physics. IBM journal of Research and Development, 11(2), pp.215-234.
NB: Richard Courant was a doctoral student and assistant of David Hilbert.

Stability criterion

- For $\theta \geq 1/2$ the integration is unconditionally stable
- Courant-Friedrichs-Lewy[1,2] or CFL condition
  the signal should not propagate more than one element in one time step:

$$\text{for } \theta < 1/2 : \qquad \text{for stability } \Delta t_c = Ch^2$$

[1] Courant, R.; Friedrichs, K.; Lewy, H. (1928), Über die partiellen Differenzengleichungen der mathematischen Physik (in German), Mathematische Annalen 100 (1): 32-74
[2] Courant, R., Friedrichs, K. and Lewy, H., 1967. On the partial difference equations of mathematical physics. IBM journal of Research and Development, 11(2), pp.215-234.
NB: Richard Courant was a doctoral student and assistant of David Hilbert.

Stability criterion

- For $\theta \geq 1/2$ the integration is unconditionally stable
- Courant-Friedrichs-Lewy[1,2] or CFL condition
  the signal should not propagate more than one element in one time step:

$$\text{for } \theta < 1/2: \qquad \text{for stability } \Delta t_c = Ch^2$$

- Coefficient C depends on the maximal eigen value of $[\boldsymbol{C}]^{-1}[\boldsymbol{K}]$

[1] Courant, R.; Friedrichs, K.; Lewy, H. (1928), Über die partiellen Differenzengleichungen der mathematischen Physik (in German), Mathematische Annalen 100 (1): 32-74
[2] Courant, R., Friedrichs, K. and Lewy, H., 1967. On the partial difference equations of mathematical physics. IBM journal of Research and Development, 11(2), pp.215-234.
NB: Richard Courant was a doctoral student and assistant of David Hilbert.

Stability criterion

- For $\theta \geq 1/2$ the integration is unconditionally stable
- Courant-Friedrichs-Lewy[1,2] or CFL condition
  the signal should not propagate more than one element in one time step:

$$\text{for } \theta < 1/2: \qquad \text{for stability } \Delta t_c = Ch^2$$

- Coefficient C depends on the maximal eigen value of $[\boldsymbol{C}]^{-1}[\boldsymbol{K}]$
- Estimating the maximal eigen value by the smallest element in the system

$$\Delta t < \Delta t_c = \frac{h^2}{8\alpha(1/2-\theta)}$$

[1] Courant, R.; Friedrichs, K.; Lewy, H. (1928), Über die partiellen Differenzengleichungen der mathematischen Physik (in German), Mathematische Annalen 100 (1): 32-74
[2] Courant, R., Friedrichs, K. and Lewy, H., 1967. On the partial difference equations of mathematical physics. IBM journal of Research and Development, 11(2), pp.215-234.
NB: Richard Courant was a doctoral student and assistant of David Hilbert.

Stability criterion

- For $\theta \geq 1/2$ the integration is unconditionally stable
- Courant-Friedrichs-Lewy[1,2] or CFL condition
  the signal should not propagate more than one element in one time step:

$$\text{for } \theta < 1/2: \qquad \text{for stability } \Delta t_c = Ch^2$$

- Coefficient C depends on the maximal eigen value of $[\boldsymbol{C}]^{-1}[\boldsymbol{K}]$
- Estimating the maximal eigen value by the smallest element in the system

$$\Delta t < \Delta t_c = \frac{h^2}{8\alpha(1/2 - \theta)}$$

- The smallest element of the mesh will control the critical time step
  one more reason to be careful with your mesh (or with your integrator)

[1] Courant, R.; Friedrichs, K.; Lewy, H. (1928), Über die partiellen Differenzengleichungen der mathematischen Physik (in German), Mathematische Annalen 100 (1): 32-74
[2] Courant, R., Friedrichs, K. and Lewy, H., 1967. On the partial difference equations of mathematical physics. IBM journal of Research and Development, 11(2), pp.215-234.
NB: Richard Courant was a doctoral student and assistant of David Hilbert.

Second order differential equations

Solid dynamics: explicit integrators

- Discretized equations:

$$[M][\ddot{u}] + [C][\dot{u}] + [K][u] = [F](t)$$

with mass matrix $[M] \in \mathbb{R}^{n\times n}$,
viscous damping matrix $[C] \in \mathbb{R}^{n\times n}$,
stiffness matrix $[K] \in \mathbb{R}^{n\times n}$,
unknown displacements $[u] \in \mathbb{R}^{n}$.

Solid dynamics: explicit integrators

- Discretized equations:
$$[\boldsymbol{M}][\ddot{\boldsymbol{u}}] + [\boldsymbol{C}][\dot{\boldsymbol{u}}] + [\boldsymbol{K}][\boldsymbol{u}] = [\boldsymbol{F}](t)$$
with mass matrix $[\boldsymbol{M}] \in \mathbb{R}^{n\times n}$,
viscous damping matrix $[\boldsymbol{C}] \in \mathbb{R}^{n\times n}$,
stiffness matrix $[\boldsymbol{K}] \in \mathbb{R}^{n\times n}$,
unknown displacements $[\boldsymbol{u}] \in \mathbb{R}^{n}$.
- For explicit integrators a similar CFL condition exist: the signal propagating at speed $c_l = \sqrt{E/\rho}$ should not propagate more than the smallest element $\min\{h\}$, resulting in
$$\Delta t < \Delta t_c = \min\{h\}\sqrt{\frac{\rho}{E}}$$
- For damping matrix $[\boldsymbol{C}]$, Rayleigh damping is often employed:
$$[\boldsymbol{C}] = \mu[\boldsymbol{M}] + \lambda[\boldsymbol{K}]$$
so the damping is frequency dependent in the following way
$$\text{Amplitude} \sim \exp(-\xi t): \qquad \xi(\omega) = \frac{1}{2}\left(\frac{\mu}{\omega} + \lambda\omega\right)$$

Solid dynamics: implicit integrators

- Discretized equations:

$$[M][\ddot{u}] + [K][u] = [F](t)$$

- Quite often only "low mode" response is of interest
- So implicit (unconditionally stable) integrators are of interest

Solid dynamics: implicit integrators

- Discretized equations:
$$[M][\ddot{u}] + [K][u] = [F](t)$$

- Quite often only "low mode" response is of interest
- So implicit (unconditionally stable) integrators are of interest
- Need to control the dissipation of high modes with a parameter other than time step.
- This dissipation should not strongly affect lower modes.

HHT integrator

Hilber-Hughes-Taylor implicit integrator[1]

- Discretized equations and initial conditions:

$$[M][\ddot{u}] + [K][u] = [F](t), \quad [u]_0 = [u_0], \quad [\dot{u}]_0 = [v_0]$$

HHT integrator

Hilber-Hughes-Taylor implicit integrator[1]

- Discretized equations and initial conditions:

$$[M][\ddot u] + [K][u] = [F](t), \quad [u]_0 = [u_0], \quad [\dot u]_0 = [v_0]$$

- Integrator with three parameters α, β, γ:

$$[M][\ddot u]_{k+1} + (1+\alpha)[K][u]_{k+1} - \alpha[K][u]_k = [F]_{k+1}$$
$$[u]_{k+1} = [u]_k + \Delta t[\dot u]_k + \Delta t^2\left[(1/2-\beta)[\ddot u]_k + \beta[\ddot u]_{k+1}\right]$$
$$[\dot u]_{k+1} = [\dot u]_k + \Delta t\left[(1-\gamma)[\ddot u]_k + \gamma[\ddot u]_{k+1}\right]$$

- Where initial accelerations are initiated as

$$[\ddot u]_0 = [M]^{-1}\left([F]_0 - [K][u]_0\right)$$

[1] Hilber, H.M., Hughes, T.J.R. and Taylor, R.L. (1977) "Improved Numerical Dissipation for Time Integration Algorithms in Structural Dynamics", Earthquake Engineering and Structural Dynamics 5:283-292

Newmark ⊂ HHT

- HHT

$$[M][\ddot{u}]_{k+1} + (1+\alpha)[K][u]_{k+1} - \alpha[K][u]_k = [F]_{k+1}$$
$$[u]_{k+1} = [u]_k + \Delta t[\dot{u}]_k + \Delta t^2\left[(1/2-\beta)[\ddot{u}]_k + \beta[\ddot{u}]_{k+1}\right]$$
$$[\dot{u}]_{k+1} = [\dot{u}]_k + \Delta t\left[(1-\gamma)[\ddot{u}]_k + \gamma[\ddot{u}]_{k+1}\right]$$

Newmark ⊂ HHT

- HHT

$$[M][\ddot{u}]_{k+1} + (1+\alpha)[K][u]_{k+1} - \alpha[K][u]_k = [F]_{k+1}$$
$$[u]_{k+1} = [u]_k + \Delta t[\dot{u}]_k + \Delta t^2\left[(1/2-\beta)[\ddot{u}]_k + \beta[\ddot{u}]_{k+1}\right]$$
$$[\dot{u}]_{k+1} = [\dot{u}]_k + \Delta t\left[(1-\gamma)[\ddot{u}]_k + \gamma[\ddot{u}]_{k+1}\right]$$

- Setting $\alpha = 0$ results in a family of *Newmark* integrators (the most common in FEM)

$$[M][\ddot{u}]_{k+1} + [K][u]_{k+1} = [F]_{k+1}$$
$$[u]_{k+1} = [u]_k + \Delta t[\dot{u}]_k + \Delta t^2\left[(1/2-\beta)[\ddot{u}]_k + \beta[\ddot{u}]_{k+1}\right]$$
$$[\dot{u}]_{k+1} = [\dot{u}]_k + \Delta t\left[(1-\gamma)[\ddot{u}]_k + \gamma[\ddot{u}]_{k+1}\right]$$

Newmark ⊂ HHT

- HHT

$$[M][\ddot{u}]_{k+1} + (1+\alpha)[K][u]_{k+1} - \alpha[K][u]_k = [F]_{k+1}$$
$$[u]_{k+1} = [u]_k + \Delta t[\dot{u}]_k + \Delta t^2\left[(1/2-\beta)[\ddot{u}]_k + \beta[\ddot{u}]_{k+1}\right]$$
$$[\dot{u}]_{k+1} = [\dot{u}]_k + \Delta t\left[(1-\gamma)[\ddot{u}]_k + \gamma[\ddot{u}]_{k+1}\right]$$

- Setting $\alpha = 0$ results in a family of *Newmark* integrators (the most common in FEM)

$$[M][\ddot{u}]_{k+1} + [K][u]_{k+1} = [F]_{k+1}$$
$$[u]_{k+1} = [u]_k + \Delta t[\dot{u}]_k + \Delta t^2\left[(1/2-\beta)[\ddot{u}]_k + \beta[\ddot{u}]_{k+1}\right]$$
$$[\dot{u}]_{k+1} = [\dot{u}]_k + \Delta t\left[(1-\gamma)[\ddot{u}]_k + \gamma[\ddot{u}]_{k+1}\right]$$

Newmark ⊂ HHT

- HHT

$$[M][\ddot u]_{k+1} + (1+\alpha)[K][u]_{k+1} - \alpha[K][u]_k = [F]_{k+1}$$
$$[u]_{k+1} = [u]_k + \Delta t[\dot u]_k + \Delta t^2\left[(1/2-\beta)[\ddot u]_k + \beta[\ddot u]_{k+1}\right]$$
$$[\dot u]_{k+1} = [\dot u]_k + \Delta t\left[(1-\gamma)[\ddot u]_k + \gamma[\ddot u]_{k+1}\right]$$

- Setting $\alpha = 0$ results in a family of *Newmark* integrators (the most common in FEM)

$$[M][\ddot u]_{k+1} + [K][u]_{k+1} = [F]_{k+1}$$
$$[u]_{k+1} = [u]_k + \Delta t[\dot u]_k + \Delta t^2\left[(1/2-\beta)[\ddot u]_k + \beta[\ddot u]_{k+1}\right]$$
$$[\dot u]_{k+1} = [\dot u]_k + \Delta t\left[(1-\gamma)[\ddot u]_k + \gamma[\ddot u]_{k+1}\right]$$

  - If $\gamma = 1/2$ – no numerical dissipation

Newmark ⊂ HHT

- HHT

$$[M][\ddot u]_{k+1} + (1+\alpha)[K][u]_{k+1} - \alpha[K][u]_k = [F]_{k+1}$$
$$[u]_{k+1} = [u]_k + \Delta t[\dot u]_k + \Delta t^2\left[(1/2-\beta)[\ddot u]_k + \beta[\ddot u]_{k+1}\right]$$
$$[\dot u]_{k+1} = [\dot u]_k + \Delta t\left[(1-\gamma)[\ddot u]_k + \gamma[\ddot u]_{k+1}\right]$$

- Setting $\alpha = 0$ results in a family of *Newmark* integrators (the most common in FEM)

$$[M][\ddot u]_{k+1} + [K][u]_{k+1} = [F]_{k+1}$$
$$[u]_{k+1} = [u]_k + \Delta t[\dot u]_k + \Delta t^2\left[(1/2-\beta)[\ddot u]_k + \beta[\ddot u]_{k+1}\right]$$
$$[\dot u]_{k+1} = [\dot u]_k + \Delta t\left[(1-\gamma)[\ddot u]_k + \gamma[\ddot u]_{k+1}\right]$$

  - If $\gamma = 1/2$ – no numerical dissipation
  - If $\gamma > 1/2$ – some numerical dissipation

Newmark ⊂ HHT

- HHT

$$[M][\ddot{u}]_{k+1} + (1+\alpha)[K][u]_{k+1} - \alpha[K][u]_k = [F]_{k+1}$$
$$[u]_{k+1} = [u]_k + \Delta t[\dot{u}]_k + \Delta t^2\left[(1/2-\beta)[\ddot{u}]_k + \beta[\ddot{u}]_{k+1}\right]$$
$$[\dot{u}]_{k+1} = [\dot{u}]_k + \Delta t\left[(1-\gamma)[\ddot{u}]_k + \gamma[\ddot{u}]_{k+1}\right]$$

- Setting $\alpha = 0$ results in a family of *Newmark* integrators (the most common in FEM)

$$[M][\ddot{u}]_{k+1} + [K][u]_{k+1} = [F]_{k+1}$$
$$[u]_{k+1} = [u]_k + \Delta t[\dot{u}]_k + \Delta t^2\left[(1/2-\beta)[\ddot{u}]_k + \beta[\ddot{u}]_{k+1}\right]$$
$$[\dot{u}]_{k+1} = [\dot{u}]_k + \Delta t\left[(1-\gamma)[\ddot{u}]_k + \gamma[\ddot{u}]_{k+1}\right]$$

  - If $\gamma = 1/2$ – no numerical dissipation
  - If $\gamma > 1/2$ – some numerical dissipation
  - β has to verify $\beta > (\gamma + 1/2)^2/4$

Analysis I

- Consider a single DOF $u(t) : u_1, u_2, \ldots$

- Consider a single DOF $u(t) : u_1, u_2, \dots$
- Introduce a vector

$$[X] = \{u, \Delta t\dot{u}, \Delta t^2\ddot{u}\}^\top$$

Analysis I

- Consider a single DOF $u(t) : u_1, u_2, \ldots$
- Introduce a vector

$$[\boldsymbol{X}] = \{u, \Delta t\dot{u}, \Delta t^2\ddot{u}\}^\top$$

- In absence of forcing $F = 0$, we get

$$[\boldsymbol{X}]_{n+1} = [A]\,[\boldsymbol{X}]_n$$

where $[A]$ is the *amplification matrix* determining stability and accuracy.

Analysis I

- Consider a single DOF $u(t) : u_1, u_2, \dots$
- Introduce a vector

$$[\boldsymbol{X}] = \{u, \Delta t\dot{u}, \Delta t^2\ddot{u}\}^\top$$

- In absence of forcing $F = 0$, we get

$$[\boldsymbol{X}]_{n+1} = [\boldsymbol{A}]\,[\boldsymbol{X}]_n$$

  where $[\boldsymbol{A}]$ is the *amplification matrix* determining stability and accuracy.
- Eigenvectors of the matrix can be found as:

$$\det([\boldsymbol{A}] - \lambda[\boldsymbol{I}]) = \lambda^3 - 2A_1\lambda^2 + A_2\lambda - A_3 = 0$$

  where $A_1 = \mathrm{tr}([\boldsymbol{A}])$, $\quad A_2 = \text{sum of principal minors},\quad A_3 = \det([\boldsymbol{A}])$

Analysis I

- Consider a single DOF $u(t) : u_1, u_2, \ldots$
- Introduce a vector

$$[\boldsymbol{X}] = \{u, \Delta t \dot{u}, \Delta t^2 \ddot{u}\}^\top$$

- In absence of forcing $F = 0$, we get

$$[\boldsymbol{X}]_{n+1} = [\boldsymbol{A}]\,[\boldsymbol{X}]_n$$

  where $[\boldsymbol{A}]$ is the *amplification matrix* determining stability and accuracy.
- Eigenvectors of the matrix can be found as:

$$\det([\boldsymbol{A}] - \lambda[\boldsymbol{I}]) = \lambda^3 - 2A_1\lambda^2 + A_2\lambda - A_3 = 0$$

  where $A_1 = \mathrm{tr}([\boldsymbol{A}]), \quad A_2 = \text{sum of principal minors}, \quad A_3 = \det([\boldsymbol{A}])$
- Spectral radius

$$\rho = \max_i\{\lambda_i\}$$

- By repetitive use of $[X]_{n+1} = [A]\,[X]_n$ and eliminating $\Delta t\dot u, \Delta t^2\ddot u$

$$u_{n+1} - 2A_1 u_n + A_2 u_{n-1} - A_3 u_{n-2} = 0$$

- By repetitive use of $[X]_{n+1} = [A]\,[X]_n$ and eliminating $\Delta t\dot{u}, \Delta t^2\ddot{u}$

$$u_{n+1} - 2A_1 u_n + A_2 u_{n-1} - A_3 u_{n-2} = 0$$

- Explicit form of the amplification matrix:

$$[A] = \frac{1}{D}\begin{bmatrix} 1+\alpha\beta\Omega^2 & 1 & 1/2-\beta \\ -\gamma\Omega^2 & 1-(1+\alpha)(\gamma-\beta)\Omega^2 & 1-\gamma-(1+\alpha)(1/2\gamma-\beta)\Omega^2 \\ -\Omega^2 & -(1+\alpha)\Omega^2 & -(1+\alpha)(1/2-\beta)\Omega^2 \end{bmatrix}$$

where

$$D = 1 + (1+\alpha)\beta\Omega^2$$
$$\Omega = \omega\Delta t$$
$$\omega = \sqrt{K/M}$$

Analysis III

- By fixing α we can select a sub-family of HHT integrators with

$$\beta = (1-\alpha)^2/4, \quad \gamma = 1/2 - \alpha$$

Analysis III

- By fixing α we can select a sub-family of HHT integrators with

$$\beta = (1-\alpha)^2/4, \quad \gamma = 1/2 - \alpha$$

- Then invariants of the amplification matrix:

$$\begin{cases} A_1 = 1 - \Omega^2/(2D) + A_3/2 \\ A_2 = 1 + 2A_3 \\ A_3 = \alpha(1+\alpha)^2\Omega^2/(4D) \end{cases}$$

where D becomes $D = 1 + (1+\alpha)(1-\alpha)^2\Omega^2/4$

Analysis III

- By fixing α we can select a sub-family of HHT integrators with

$$\beta = (1-\alpha)^2/4, \quad \gamma = 1/2 - \alpha$$

- Then invariants of the amplification matrix:

$$\begin{cases} A_1 = 1 - \Omega^2/(2D) + A_3/2 \\ A_2 = 1 + 2A_3 \\ A_3 = \alpha(1+\alpha)^2\Omega^2/(4D) \end{cases}$$

  where D becomes $D = 1 + (1+\alpha)(1-\alpha)^2\Omega^2/4$
- So eigenvalues could be found from:

$$(\lambda - A_3)(\lambda - 1)^2 + \Omega^2\lambda^2/D = 0$$

Analysis IV

- In the limit $\Omega \to \infty$

$$\left[(1-\alpha)(1-\alpha)^2\lambda - \alpha(1+\alpha)^2\right](\lambda-1)^2 + 4\lambda^2 = 0$$

- In the limit $\Omega \to \infty$

$$\left[(1-\alpha)(1-\alpha)^2\lambda - \alpha(1+\alpha)^2\right](\lambda-1)^2 + 4\lambda^2 = 0$$

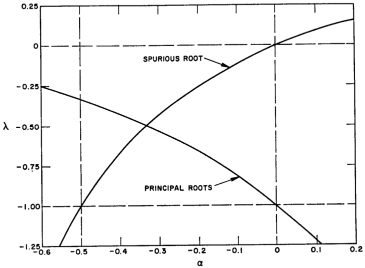


Figure 1. Eigenvalues of the amplification matrix in the limit $\Delta t/T \to \infty$ *vs* α

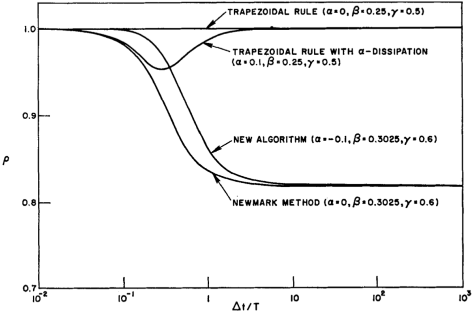
Figure from[1]

$\Rightarrow$ HHT integrator is stable if $-1/2 \le \alpha \le 0$

[1] Hilber, H.M., Hughes, T.J.R. and Taylor, R.L. (1977) ”Improved Numerical Dissipation for Time Integration Algorithms in Structural Dynamics”, Earthquake Engineering and Structural Dynamics 5:283-292

Comparison

(1) Trapezoidal rule $\alpha = 0, \beta = 0.25, \gamma = 0.5$
(2) Trapezoidal rule with damping $\alpha = 0.1, \beta = 0.25, \gamma = 0.5$
(3) Newmark with γ damping $\alpha = 0, \beta = 0.3025, \gamma = 0.6$
(4) HHT $\alpha = -0.1, \beta = 0.3025, \gamma = 0.6$



Spectral radii ρ[1]
$T = 2\pi/\omega$

[1] Hilber, H.M., Hughes, T.J.R. and Taylor, R.L. (1977) "Improved Numerical Dissipation for Time Integration Algorithms in Structural Dynamics", Earthquake Engineering and Structural Dynamics 5:283-292

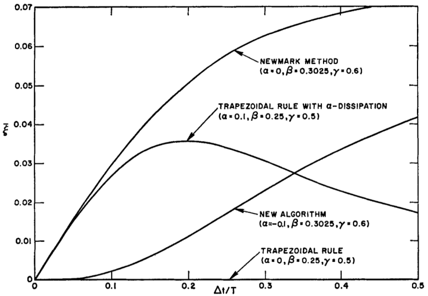
Comparison

(1) Trapezoidal rule $\alpha = 0, \beta = 0.25, \gamma = 0.5$

(2) Trapezoidal rule with damping $\alpha = 0.1, \beta = 0.25, \gamma = 0.5$

(3) Newmark with γ damping $\alpha = 0, \beta = 0.3025, \gamma = 0.6$

(4) HHT $\alpha = -0.1, \beta = 0.3025, \gamma = 0.6$



Damping factor[1] $\bar\xi : u_n \sim \exp(-\bar\xi\bar\omega t_n)$

$T = 2\pi/\omega$

[1] Hilber, H.M., Hughes, T.J.R. and Taylor, R.L. (1977) "Improved Numerical Dissipation for Time Integration Algorithms in Structural Dynamics", Earthquake Engineering and Structural Dynamics 5:283-292

Examples

Merci de votre attention !