3 FINITE DIFFERENCE METHOD

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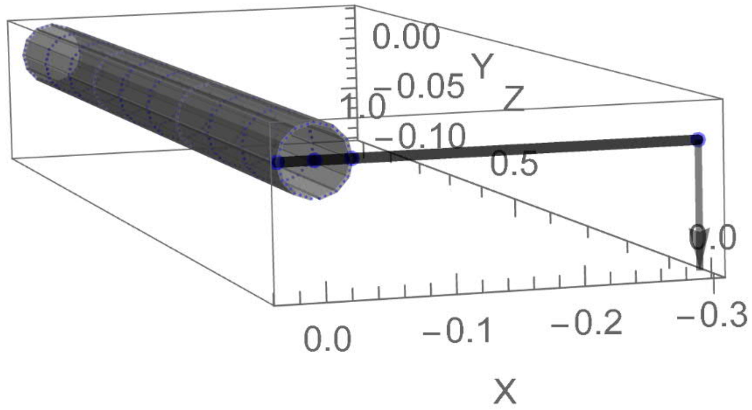
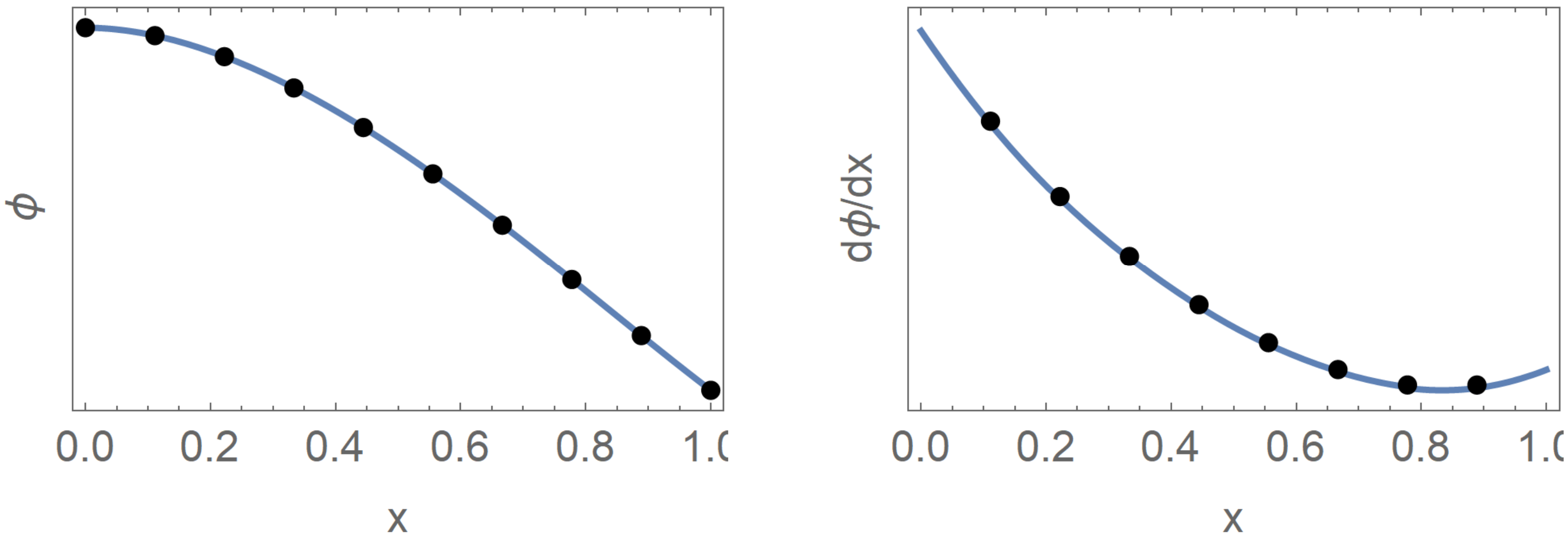
SIMULATION EXPERIMENT



The outcome of the simulation experiment is the dataset $\{(x_0, \phi_0), (x_1, \phi_1), \ldots, (x_n, \phi_n)\}$ consisting of axial rotation angles on a regular grid on the axis. Processing of data is required to find the derivative of the rotation with respect to the axial coordinate.



Interpolation of the dataset gives a continuous representation (in blue on the left) of continuous derivative (in blue on the right). The dataset (in black on the left) can also be used directly to find the dataset for derivates (in black on the righ). The outcomes differ but not much.

PROCESSING OF DATA

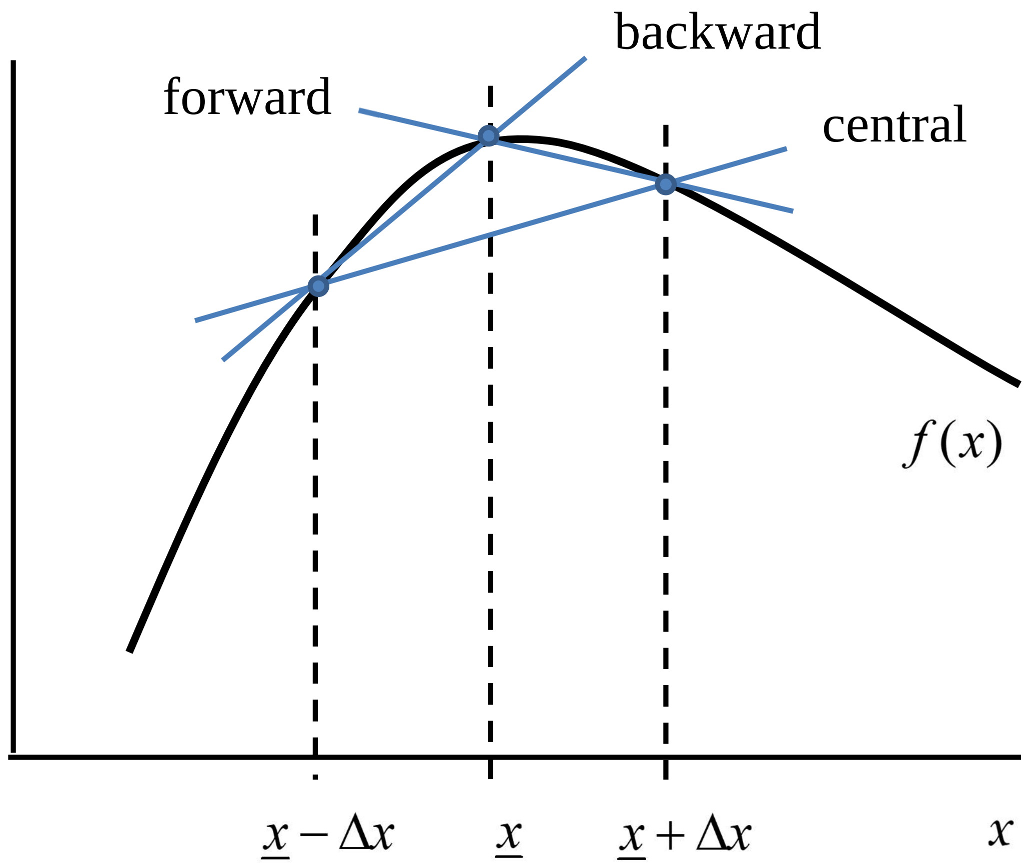
In a typical design, dataset of an experiment $\{\ldots,(x_i, f_i),(x_{i+1}, f_{i+1}),\ldots\}$ is considered as sampling of the underlying continuous *dependent quantity* $f(x)$ at values $\{\ldots, x_i, x_{i+1},\ldots\}$ of the *independent quantity* x. In further processing of data, one may

- □ use the dataset to find a continuous approximation $g(x)$ to $f(x)$. Thereafter finding the value at any point, calculation of derivatives, integration etc. with *generic methods* is possible.

- □ use the dataset directly to find, e.g., derivatives at the sampling points, integrals, etc. using *dedicated methods* like difference approximations and quadratures (numerical integration).

Although the details of the methods differ, the results at the sampling points may not differ too much from the engineering viewpoint.

3.1 APPROXIMATION TO DERIVATIVES



Judging from the figure, central difference $f'(\underline{x}) = [-f(\underline{x}-\Delta x) + f(\underline{x}+\Delta x)]/(2\Delta x)$ gives the best approximation to the first derivative at $\underline{x}$.

TAYLOR'S THEOREM

Taylor's series with the remainder term is an important tool in numerical methods. Theorem tells how to approximate a function in some neighborhood of a point by a polynomial (below $f^{(i)}(x)$ denotes the i:th derivative of $f(x)$)

1D: $$f(x+\Delta x) = f(x) + \frac{1}{1!} f^{(1)}(x)\Delta x + \ldots + \frac{1}{(n-1)!} f^{(n-1)}(x)\Delta x^{n-1} + \frac{1}{n!} f^{(n)}(\xi)\Delta x^n$$

nD: $$f(x+\mathrm{a}) = \sum_{i=0}^{n-1} \frac{1}{i!}(\Delta\vec{x}\cdot\nabla)^i f(\vec{x}) + \frac{1}{n!}[(\Delta\vec{x}\cdot\nabla)^n f(\vec{x})]_{\vec{x}=\vec{\xi}}$$

Theorem assumes existence of the n:th derivative. In the remainder term, ξ is some point to the interval which is different in each occurrence. In the finite difference method, approximations to derivatives in terms function values at certain points are often derived with the aid of the theorem.

DIFFERENCE APPROXIMATIONS TO $f'(x)$

For function $f(x)$ values on a regularly spaced grid of resolution Δx, an order k difference approximation to $f'(x)$ on the grid points has a remainder term proportional to Δx^k. The approximation is exact to a polynomial $f(x)$ of degree k.

Type	$f'(x)$	Order
Backward	$\dfrac{f(x)-f(x-\Delta x)}{\Delta x}$	1
Forward	$\dfrac{-f(x)+f(x+\Delta x)}{\Delta x}$	1
Central	$\dfrac{-f(x-\Delta x)+f(x+\Delta x)}{2\Delta x}$	2
Central	$\dfrac{f(x-2\Delta x)-8f(x-\Delta x)+8f(x+\Delta x)-f(x+2\Delta x)}{12\Delta x}$	4

Difference approximations follow from the Taylor's representation truncated at certain term and written for points $x \pm k\Delta x$. The central differences can be derived using the versions

$$f(x+\Delta x) = f(x) + f'(x)\Delta x + \frac{1}{2} f''(x)\Delta x^2 + \frac{1}{6} f^{(3)}(\xi_1)\Delta x^3,$$

$$f(x-\Delta x) = f(x) - f'(x)\Delta x + \frac{1}{2} f''(x)\Delta x^2 - \frac{1}{6} f^{(3)}(\xi_2)\Delta x^3.$$

Adding and subtracting on both sides, rearranging, and dividing with an appropriate power of Δx

$$\frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} = f'(x) + \frac{1}{12}[f^{(3)}(\xi_1) - f^{(3)}(\xi_2)]\Delta x^2,$$

$$\frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2} = f''(x) + \frac{1}{6}[f^{(3)}(\xi_1) - f^{(3)}(\xi_2)]\Delta x.$$

DIFFERENCE APPROXIMATIONS TO $f''(x)$

Type	$f''(x)$	Order
Backward	$\dfrac{f(x-2\Delta x)-2f(x-\Delta x)+f(x)}{\Delta x^2}$	1
Forward	$\dfrac{f(x)-2f(x+\Delta x)+f(x+2\Delta x)}{\Delta x^2}$	1
Central	$\dfrac{f(x-\Delta x)-2f(x)+f(x+\Delta x)}{\Delta x^2}$	2
Central	$\dfrac{-f(x-2\Delta x)+16f(x-\Delta x)-30f(x)+16f(x+\Delta x)-f(x+2\Delta x)}{12\Delta x}$	4

Difference approximations follow from the Taylor's representation truncated at certain term and written for points $x \pm k\Delta x$. Backward differences can be obtained by using the versions

$$2f(x-\Delta x) = 2f(x) - 2f'(x)\Delta x + f''(x)\Delta x^2 - \frac{1}{3} f^{(3)}(\xi_1)\Delta x^3,$$

$$-f(x-2\Delta x) = -f(x) + 2f'(x)\Delta x - 2f''(x)\Delta x^2 + \frac{4}{3} f^{(3)}(\xi_2)\Delta x^3.$$

Adding and subtracting on both sides, rearranging, and dividing with an appropriate power of Δx

$$2f(x-\Delta x) - f(x-2\Delta x) = f(x) - f''(x)\Delta x^2 - \frac{1}{3} f^{(3)}(\xi_1)\Delta x^3 + \frac{4}{3} f^{(3)}(\xi_2)\Delta x^3,$$

$$2f(x-\Delta x) - f(x-2\Delta x) = f(x) - f''(x)\Delta x^2 - \frac{1}{3} f^{(3)}(\xi_1)\Delta x^3 + \frac{4}{3} f^{(3)}(\xi_2)\Delta x^3$$

EXAMPLE A straightforward way to construct difference formulas for derivatives uses a polynomial interpolant to dataset $\{\ldots,(x_i, f_i),(x_{i+1}, f_{i+1}),\ldots\}$ and derivatives of the interpolant at the grid points. As an example, let us consider the interpolant $p(x)$ to $\{(x_{i-1}, f_{i-1}),(x_i, f_i),(x_{i+1}, f_{i+1})\}$ to find the difference approximations to the first and second derivatives at x_i by calculating the derivatives of the interpolant at that point. Assume a regular grid of points of spacing Δx.

Answer $f_i' = p'(x_i) = \dfrac{-f_{i-1} + f_{i+1}}{2\Delta x}$ and $f_i'' = p''(x_i) = \dfrac{f_{i-1} - 2f_i + f_{i+1}}{\Delta x^2}$

The well-known Lagrange interpolation polynomial $p_n(x)$ of degree n and its error formula are for dataset $\{(x_0, f_0),(x_1, f_1),\ldots(x_n, f_n)\}$

$$p_n(x) = \sum_{i\in\{0,1,\ldots,n\}} f_i \Pi_{j\in\{0,1,\ldots i-1,i+1,\ldots,n\}} \frac{x - x_j}{x_i - x_j},$$

$$f(x) - p_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi)\Pi_{i\in\{0,1,\ldots,n\}}(x - x_i) \ .$$

Notice the removal of index i in the product term inside the sum of the interpolation formula. With dataset $\{(x_{i-1}, f_{i-1}),(x_i, f_i),(x_{i+1}, f_{i+1})\}$

$$p(x) = f_{i-1}\frac{x - x_i}{x_{i-1} - x_i}\frac{x - x_{i+1}}{x_{i-1} - x_{i+1}} + f_i\frac{x - x_{i-1}}{x_i - x_{i-1}}\frac{x - x_{i+1}}{x_i - x_{i+1}} + f_{i+1}\frac{x - x_{i-1}}{x_{i+1} - x_{i-1}}\frac{x - x_i}{x_{i+1} - x_i}.$$

Selection $x_i = i\Delta x$ and representation with monomials of increasing powers, which is more convenient in calculation of derivatives, gives the (equivalent) form

$$p(x) = f_i - \frac{x}{2\Delta x}(-f_{i-1} + f_{i+1}) + \frac{x^2}{2\Delta x^2}(f_{i-1} - 2f_i + f_{i+1}).$$

Therefore, the calculation with the interpolant to the dataset implies the well-known 2:nd order accurate difference approximations to the first and second derivatives

$$f_i' = p'(0) = \frac{-f_{i-1} + f_{i+1}}{2\Delta x} \quad \text{and} \quad f_i'' = p''(0) = \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta x^2}.$$

The power Δx^2 in the remainder term can be verified by a direct calculation with the remainder expression.

DIFFERENCE STENCILS

Derivative	Accuracy	−5	−4	−3	−2	−1	0	1	2	3	4	5
1	2					−1/2	0	1/2				
	4				1/12	−2/3	0	2/3	−1/12			
	6			−1/60	3/20	−3/4	0	3/4	−3/20	1/60		
	8		1/280	−4/105	1/5	−4/5	0	4/5	−1/5	4/105	−1/280	
2	2					1	−2	1				
	4				−1/12	4/3	−5/2	4/3	−1/12			
	6			1/90	−3/20	3/2	−49/18	3/2	−3/20	1/90		
	8		−1/560	8/315	−1/5	8/5	−205/72	8/5	−1/5	8/315	−1/560	
3	2				−1/2	1	0	−1	1/2			
	4			1/8	−1	13/8	0	−13/8	1	−1/8		
	6		−7/240	3/10	−169/120	61/30	0	−61/30	169/120	−3/10	7/240	
4	2				1	−4	6	−4	1			
	4			−1/6	2	−13/2	28/3	−13/2	2	−1/6		
	6		7/240	−2/5	169/60	−122/15	91/8	−122/15	169/60	−2/5	7/240	
5	2			−1/2	2	−5/2	0	5/2	−2	1/2		
	4		1/6	−3/2	13/3	−29/6	0	29/6	−13/3	3/2	−1/6	
	6	−13/288	19/36	−87/32	13/2	−323/48	0	323/48	−13/2	87/32	−19/36	13/288

https://en.wikipedia.org/wiki/Finite_difference_coefficient

3.2 FINITE DIFFERENCE METHOD

Finite Difference Method is a numerical technique for solving ordinary and partial differential equations by approximating derivatives with finite difference formulas. If applied with a regular grid to the string and bar models, the discrete equations by the FDM

Interior $\frac{k'}{h^2}(a_{i-1} - 2a_i + a_{i+1}) + f' = m'\ddot{a}_i \quad i \in \{1, 2, \ldots, n-1\}$

Boundary $a_0 = \underline{a}_0$ or $-\frac{k'}{h}(a_1 - a_0) = \underline{F}_0$ and $a_n = \underline{a}_n$ or $\frac{k'}{h}(a_n - a_{n-1}) = \underline{F}_n$

Initial conditions $a_i - g_i = 0$ and $\dot{a}_i - h_i = 0 \quad i \in \{1, 2, \ldots, n-1\}$

Then, the outcome is a set of Ordinary Differential Equations of the same type as by the Particle Surrogate Method. Therefore, the matrix and difference equation techniques for PSM also apply to FDM.

Continuum model of bar or string of known displacement or loading at the end points and known initial position and velocity is given by equations

$$k'\frac{\partial^2 a}{\partial x^2}+f'=m'\frac{\partial^2 a}{\partial t^2} \quad x\in\Omega \quad t>0$$

$$a=\underline{a} \ \text{ or } \ n_x(k'\frac{\partial a}{\partial x})=\underline{F} \quad x\in\partial\Omega \quad t>0,$$

$$a=g \quad \text{and} \quad \frac{\partial a}{\partial t}=h \quad x\in\Omega \quad t=0.$$

By using the 2:nd order accurate central difference approximation for the second partial derivative in the equation of the motion and 1:st order accurate difference approximation for the derivative in the boundary condition, one obtains

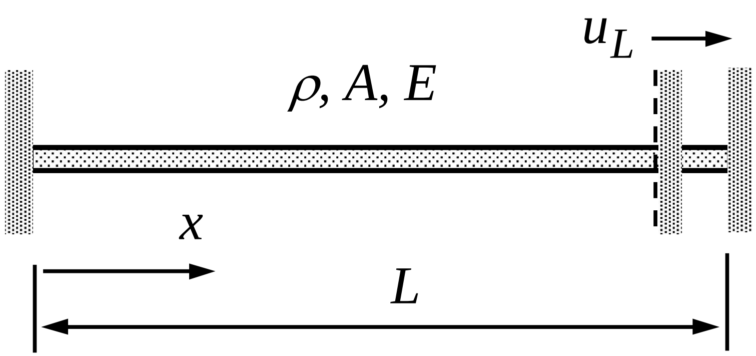
$$\frac{k'}{h^2}(a_{i-1}-2a_i+a_{i+1})+f'=m'\ddot{a}_i \quad i\in\{1,2,\ldots,n-1\}$$

$$a_0 = \underline{a}_0 \text{ or } -\frac{k'}{h}(a_1 - a_0) = \underline{F}_0 \text{ and } a_n = \underline{a}_n \text{ or } \frac{k'}{h}(a_n - a_{n-1}) = \underline{F}_n$$

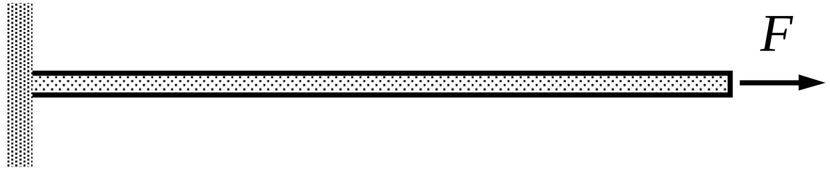
$$w_i - g_i = 0 \quad \text{and} \quad \dot{w}_i - h_i = 0 \quad i \in \{1, 2, \ldots, n-1\} \quad t = 0.$$

Multiplication of both sides of the equation of motion by h (here spacing of the grip points) gives the final form which differs only in the equations for the boundary points from those for the Particle Surrogate Method. As the starting point of FDM are the differential equations of the continuum model, e.g., point forces, point masses etc. not located at the boundaries need to be represented correctly in the continuum model before the use of FDM. At non-regular points, the differential equation should be replaced by jump conditions implied by the first principles of mechanics. Also, the grid should be adjusted to have a grid point at positions of point forces and masses.

1st ORDER BOUNDARY CONDITIONS FOR BAR



$$u_0 = 0, \quad u_n - \underline{u} = 0$$

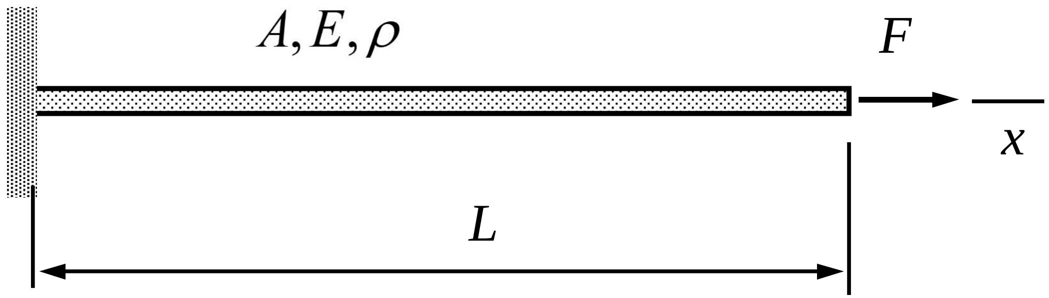


$$u_0 = 0, \quad EA\frac{u_n - u_{n-1}}{h} - F_n = 0$$

$$u_0 = 0, \quad EA\frac{u_n - u_{n-1}}{h} + m\ddot{u}_n = 0$$

$$u_0 = 0, \quad EA\frac{u_n - u_{n-1}}{h} + ku_n = 0$$

EXAMPLE The elastic bar shown is loaded by a point force at the right end. The left end is fixed. Determine the stationary solution displacement using the Finite Difference Method on a regular grid $i \in \{0,1,\ldots,n\}$ on the solution domain of length L. Material properties and cross-sectional area are constants. What is limit solution when $n \to \infty$ and $h = L/n$?



Answer $u_i = ih\dfrac{F}{EA} = x_i \dfrac{F}{EA}$, limit solution $u(x) = x\dfrac{F}{EA}$

Using the 2:nd order accurate central difference approximation to the second derivative in the equilibrium equation for typical grid point $i \in \{1,2,\ldots,n-1\}$ and first order accurate approximation to the first derivative in the boundary condition at the loaded end

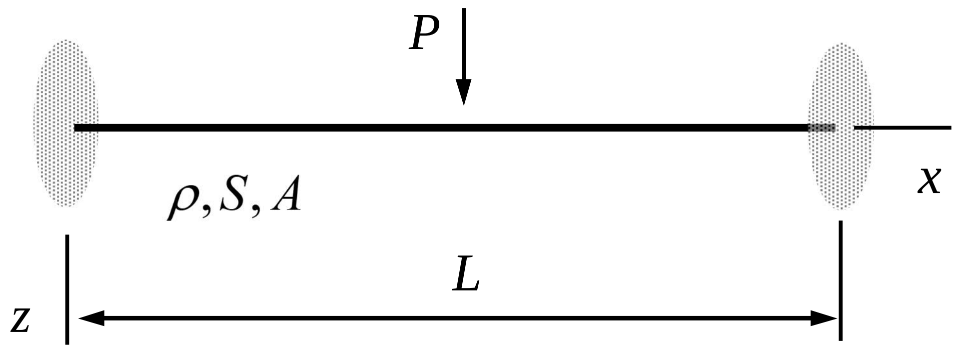
$$EA\left(\frac{u_{i-1} - 2u_i + u_{i+1}}{h^2}\right) = 0 \quad i \in \{1,2,\ldots,n-1\}, \;\; u_0 = 0 \;, \;\; \text{and} \;\; EA\frac{u_n - u_{n-1}}{h} = F \,.$$

When substituted into the difference equation, the solution trial $u_i = ar^i$ implies the condition $1 - 2r + r^2 = (1-r)^2 = 0$ so the generic solution is $u_i = a + bi$ (double root $r = 1$) . The two constants follow from equations for the boundary points

$$u_0 = a = 0 \quad \text{and} \quad EA\frac{a + bn - a - b(n-1)}{h} = F \quad \Leftrightarrow \quad a = 0 \;\; \text{and} \;\; b = \frac{hF}{EA}.$$

Hence $u_i = ih\dfrac{F}{EA} = x_i\dfrac{F}{EA}$ (in the limit $u(x) = x\dfrac{F}{EA}$). 🡸

EXAMPLE A string of length L, tightening S, cross-sectional area A, and density ρ, is loaded by a point force P at its center point. If the ends are fixed and the initial geometry without loading is straight, find the solution to the transverse displacement as function of x using the finite difference method on a regular grid of three points $i \in \{0,1,2\}$.



Answer $w_1 = \dfrac{PL}{4S}$

The boundary value problem is given by equilibrium equations for the regular interior points, jump conditions at the center point (non-regular point due to the point force), and boundary conditions for the end points

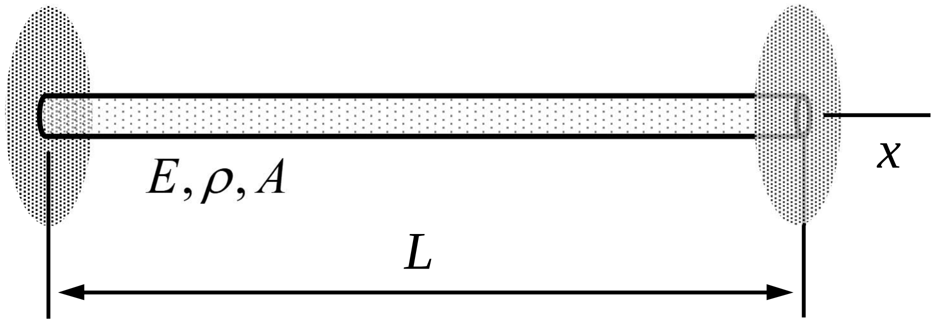
$$S\frac{d^2w}{dx^2}=0 \quad x\in]0,\frac{L}{2}[\quad \text{or} \quad x\in]\frac{L}{2},L[,$$

$$S\left[\!\left[\frac{dw}{dx}\right]\!\right]+P=0\ ,\ [\![w]\!]=0 \quad x=\frac{L}{2},\ \text{ and } w(x)=0 \quad x\in\{0,L\}.$$

As the end points are fixed and there is a discontinuity at the midpoint, only the jump condition applies. Let us use the first order accurate backward and forward two-point difference approximations to the left and right derivatives, to get ($w_0=w_2=0$ and $\Delta x=L/2$):

$$S(\frac{w_2-w_1}{\Delta x}-\frac{w_1-w_0}{\Delta x})+P=0 \quad \Rightarrow \quad w_1=\frac{PL}{4S}.$$

EXAMPLE Write the equations of motion for the free vibrations of the bar shown by using FDM. Use the matrix formulation on a regular grid with $i \in \{0,1,2,3\}$. Material properties E, ρ and the cross-sectional area A are constants. Also, determine the two lowest angular velocities and the corresponding modes of the free vibrations.



Answer $\dfrac{EA}{h^2}\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}\begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix} + \rho A \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{Bmatrix} \ddot{u}_1 \\ u_2 \end{Bmatrix} = 0$ where $h = \dfrac{L}{3}$

The equations for the points inside the domain, as given by the 2:nd order accurate central difference approximation to the second derivative (with respect to x), are

$$u_0 = 0 \ , \ \frac{EA}{h^2}(u_0 - 2u_1 + u_2) = \rho A\ddot{u}_1 \ , \ \frac{EA}{h^2}(u_1 - 2u_2 + u_3) = \rho A\ddot{u}_2, \text{ and } \ u_3 = 0.$$

In matrix notation and $k = EA/h$, $m = \rho Ah$, and $h = L/3$, the equations for points 1 and 2 are (when the known displacements at the boundary points are used there)

$$k\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}\begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix} + m\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{Bmatrix} \ddot{u}_1 \\ u_2 \end{Bmatrix} = 0. \quad \Leftarrow$$

Frequencies and modes of the free vibrations follow with the trial solution $\mathbf{u} = \mathbf{A}\exp(\mathrm{i}\omega t)$. Using the notation $\lambda = \omega^2 m/k$

$$(\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} - \lambda\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix})\begin{Bmatrix} A_1 \\ A_2 \end{Bmatrix} = 0 \ .$$

The homogeneous linear equation system can yield a non-zero solution to the mode only if the matrix in parenthesis is singular so its determinant needs to vanish

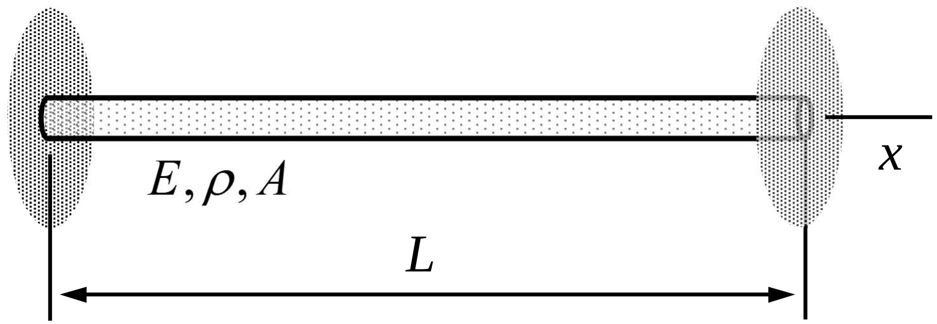
$$\det\begin{bmatrix} 2-\lambda & -1 \\ -1 & 2-\lambda \end{bmatrix} = (2-\lambda)^2 - 1 = 0 \quad \Rightarrow \quad \lambda_1 = 1 \text{ or } \lambda_2 = 3.$$

Knowing the possible λ:s and also the angular velocities from $\lambda = \omega^2 m / k$, solution to the modes are given by the linear equation systems:

$$\lambda_1 = 1: \quad \omega_1 = \sqrt{\lambda \frac{k}{m}} \text{ and } \begin{bmatrix} 2-1 & -1 \\ -1 & 2-1 \end{bmatrix} \begin{Bmatrix} A_1 \\ A_2 \end{Bmatrix} = 0 \quad \text{so} \quad (\omega_1, \mathbf{A}_1) = (\sqrt{\frac{k}{m}}, \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}).$$

$$\lambda_2 = 3: \quad \omega_2 = \sqrt{3 \frac{k}{m}} \text{ and } \begin{bmatrix} 2-3 & -1 \\ -1 & 2-3 \end{bmatrix} \begin{Bmatrix} A_1 \\ A_2 \end{Bmatrix} = 0 \quad \text{so} \quad (\omega_2, \mathbf{A}_2) = (\sqrt{3 \frac{k}{m}}, \begin{Bmatrix} 1 \\ -1 \end{Bmatrix}).$$

EXAMPLE Consider the free vibrations of the bar shown, when material properties E, ρ and cross-sectional area A are constants. Use finite difference method with a second order accurate central difference approximation to find the displacement as the function time on a regular grid $i \in \{0,1,\ldots,n\}$ when the initial displacement and velocity are $u_i = \sum_{k\in\{1,2,\ldots,n-1\}} \alpha_k \sin(k\pi i/n)$ and $\dot{u}_i = 0$ $i \in \{0,1,\ldots,n\}$ respectively. Hint. Use the displacement assumption $u_i = \sum_{k\in\{1,2,\ldots,n-1\}} a_k(t)\sin(k\pi i/n)$



Answer $u_i(t) = \sum_{k\in\{1,2,\ldots,n-1\}} \alpha_k \cos(\omega_k t)\sin(k\pi \frac{i}{n})$ and $\omega_k = \sqrt{\frac{2E}{\rho L^2} n^2 [1-\cos(\pi \frac{k}{n})]}$

Lets start with the difference equations

$$\frac{EA}{h^2}(u_{i-1}-2u_i+u_{i+1})=\rho A\ddot{u}_i \quad \text{and} \quad u_i=0 \quad i\in\{0,n\}$$

and use the solution assumption motivated by the form of the initial condition (can be considered as the discrete fourier series of some continuous initial displacement at the grid points)

$$u_i(t)=\sum\nolimits_{k\in\{1,2,\ldots,n-1\}} a_k(t)\sin(k\pi\frac{i}{n}).$$

Notice that the number terms correspond to the number of interior grid points) $i\in\{1,2,\ldots,n-1\}$. As the differential equation is linear it is enough to consider a typical term k giving when substituted into the difference expression and second time derivative

$$u_{i-1}-2u_i+u_{i+1}=2a_k(t)[\cos(\pi\frac{k}{n})-1]\sin(k\pi\frac{i}{n}) \quad \text{and} \quad \ddot{u}_i=\sin(k\pi\frac{i}{n})\ddot{a}_k.$$

Consequently, the difference-differential equation and the initial conditions associated with the k:th term boil down to an initial value problem for the unknown $a_k(t)$ of the displacement assumption

$$\ddot{a}_k + \omega_k^2 a_k = 0 \quad t > 0 \;, \;\; a_k(0) = \alpha_k \;\text{ and }\; \dot{a}_k(0) = 0 \;\text{ where }\; \omega_k = \sqrt{\frac{2E}{\rho h^2}[1 - \cos(\pi \frac{k}{n})]}$$

whose solution is $a_k(t) = \alpha_k \cos(\omega_k t)$. Putting everything together, the solution to the vibration problem with initial displacement in terms of the discrete Fourier sine series becomes

$$u_i(t) = \sum\nolimits_{k \in \{1,2,\ldots,n-1\}} \alpha_k \cos(\omega_k t) \sin(k\pi \frac{i}{n}) \;\text{ where }\; \omega_k = \sqrt{\frac{2E}{\rho L^2} n^2 [1 - \cos(\pi \frac{k}{n})]} .$$

DISCRETE SINE SERIES

The discrete Fourier series (various forms exist) can be used to represent a list as the sum of lists of harmonic terms. For example, the sine-transformation pair for a list a_i $i \in \{1, 2, \ldots, n-1\}$ is given by

$$\alpha_j = \frac{2}{n} \sum_{i \in \{1,2,\ldots,n-1\}} \sin(j\pi \frac{i}{n}) a_i \quad j \in \{1, 2, \ldots, n-1\}$$

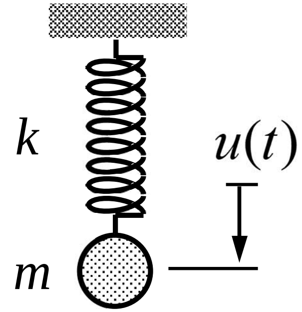
$$a_i = \sum_{j \in \{1,2,\ldots,n-1\}} \alpha_j \sin(j\pi \frac{i}{n}) \quad i \in \{1, 2, \ldots, n-1\}$$

The transformation pair is based on the orthogonality of the modes (Cronecker delta $\delta_{jl} = 1$ if $j = l$ and $\delta_{jl} = 0$ if $j \neq l$)

$$\sum_{j \in \{1,2,\ldots,n-1\}} \sin(j\pi \frac{i}{n}) \sin(l\pi \frac{i}{n}) = \delta_{jl} \frac{n}{2}.$$

3.3 TIME INTEGRATION

In time integration, the solution is sought step-by-step using a regular grid on the temporal domain $t_i = i\Delta t \;\; i \in \{0,1,\ldots\}$, where Δt is the step size. The exact one particle vibration solution to displacement and velocity at the grid points represents the generic idea of a recursive one-step time-integration method:



$$\begin{Bmatrix} u \\ \dot{u} \end{Bmatrix} = \begin{bmatrix} \cos(\omega t) & \omega^{-1}\sin(\omega t) \\ -\omega\sin(\omega t) & \cos(\omega t) \end{bmatrix} \begin{Bmatrix} g \\ h \end{Bmatrix} \text{ where } \omega = \sqrt{\frac{k}{m}} \;\; \Rightarrow$$

$$\begin{Bmatrix} u \\ \Delta t\dot{u} \end{Bmatrix}_i = \begin{bmatrix} \cos(\alpha i) & \alpha^{-1}\sin(\alpha i) \\ -\alpha\sin(\alpha i) & \cos(\alpha i) \end{bmatrix} \begin{Bmatrix} g \\ \Delta t h \end{Bmatrix} \text{ where } \alpha = \Delta t\omega = \Delta t\sqrt{\frac{k}{m}} \;\; \Rightarrow$$

$$\begin{Bmatrix} u \\ \Delta t\dot{u} \end{Bmatrix}_i = \begin{bmatrix} \cos\alpha & \alpha^{-1}\sin\alpha \\ -\alpha\sin\alpha & \cos\alpha \end{bmatrix} \begin{Bmatrix} u \\ \Delta t\dot{u} \end{Bmatrix}_{i-1} \;\; i \in \{1,2,\ldots\} \text{ and } \begin{Bmatrix} u \\ \Delta t\dot{u} \end{Bmatrix}_0 = \begin{Bmatrix} g \\ \Delta t h \end{Bmatrix}.$$

Let us consider free vibration of one particle with known position and velocity at the initial time described by the initial value problem

$$m\ddot{u} + ku = 0 \;\; t > 0, \;\; \dot{u}(0) = h, \quad u(0) = g\,.$$

The exact solutions to displacement and velocity can be expressed in the form

$$\begin{Bmatrix} u \\ \dot{u} \end{Bmatrix} = \begin{bmatrix} \cos(\omega t) & \omega^{-1}\sin(\omega t) \\ -\omega\sin(\omega t) & \cos(\omega t) \end{bmatrix} \begin{Bmatrix} g \\ h \end{Bmatrix} \text{ where } \;\omega = \sqrt{\frac{k}{m}}\,.$$

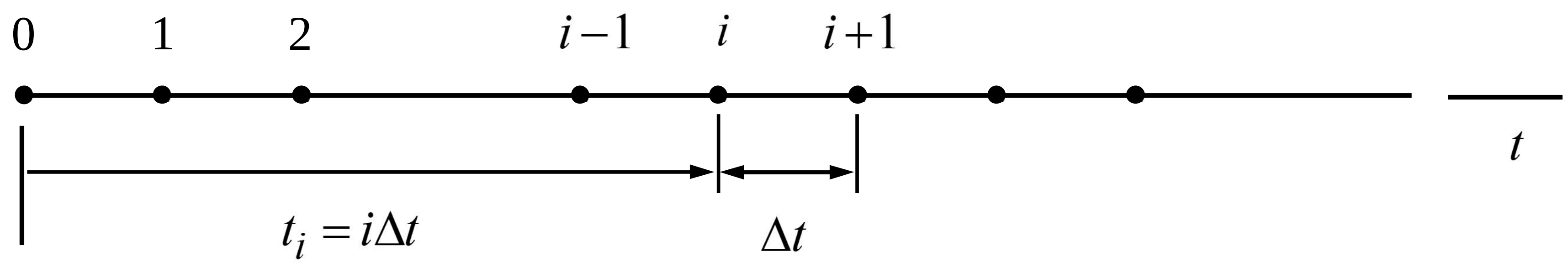
Solution at point $t_i = i\Delta t$ of the regular temporal grid

$$\begin{Bmatrix} u \\ \Delta t\dot{u} \end{Bmatrix}_i = \begin{bmatrix} \cos(\alpha i) & \alpha^{-1}\sin(\alpha i) \\ -\alpha\sin(\alpha i) & \cos(\alpha i) \end{bmatrix} \begin{Bmatrix} g \\ \Delta t h \end{Bmatrix} \text{ where } \alpha = \Delta t\omega = \Delta t\sqrt{\frac{k}{m}}\,.$$

In recursive form, initial conditions give the solution at the end of the first time-interval to be treated as the initial conditions for the next time-interval and so on.

REGULAR TEMPORAL GRID

On a regular grid, the grid points are distributed evenly. The number of the point at the origin is 0 and the numbering increases in the direction of the $t-$axis without gaps. The time intervals are referenced by their end point indices (i.e., interval i is between grid points $i-1$ and i.



As the temporal domain for an initial value problem does not have an upper bound (strictly speaking), the length of the intervals can (and often are) chosen to match the behavior of the solution (small steps for the rapid changes).

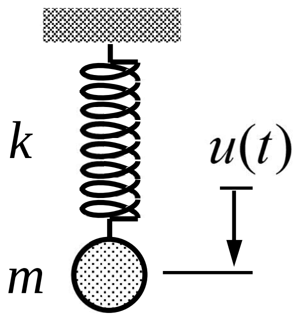
TIME INTEGRATION

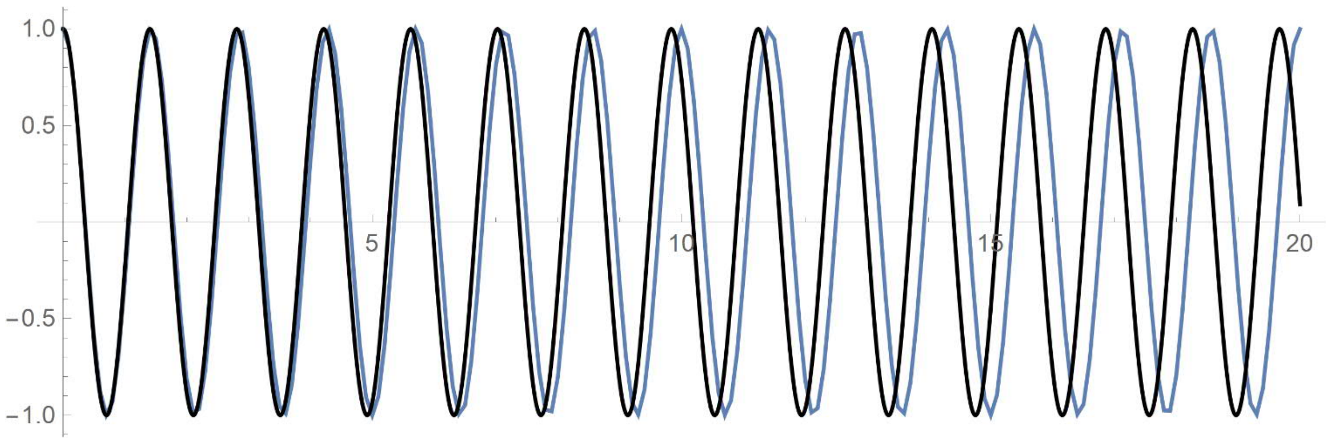
Method	Iteration $i \in \{1, 2, \ldots\}$	Initial $i = 0$
EX	$\begin{Bmatrix} a \\ \Delta t\dot{a} \end{Bmatrix}_i = \begin{bmatrix} \cos\alpha & \alpha^{-1}\sin\alpha \\ -\alpha\sin\alpha & \cos\alpha \end{bmatrix} \begin{Bmatrix} a \\ \Delta t\dot{a} \end{Bmatrix}_{i-1}$	$\begin{Bmatrix} a \\ \Delta t\dot{a} \end{Bmatrix}_0 = \begin{Bmatrix} g \\ \Delta t h \end{Bmatrix}$
CN	$\begin{Bmatrix} a \\ \Delta t\dot{a} \end{Bmatrix}_i = \frac{1}{4+\alpha^2} \begin{bmatrix} 4-\alpha^2 & 4 \\ -4\alpha^2 & 4-\alpha^2 \end{bmatrix} \begin{Bmatrix} a \\ \Delta t\dot{a} \end{Bmatrix}_{i-1}$	$\begin{Bmatrix} a \\ \Delta t\dot{a} \end{Bmatrix}_0 = \begin{Bmatrix} g \\ \Delta t h \end{Bmatrix}$
DG	$\begin{Bmatrix} a \\ \Delta t\dot{a} \end{Bmatrix}_i = \frac{2}{12+\alpha^4} \begin{bmatrix} 6-3\alpha^2 & 6-\alpha^2 \\ -6\alpha^2 & 6-3\alpha^2 \end{bmatrix} \begin{Bmatrix} a \\ \Delta t\dot{a} \end{Bmatrix}_{i-1}$	$\begin{Bmatrix} a \\ \Delta t\dot{a} \end{Bmatrix}_0 = \begin{Bmatrix} g \\ \Delta t h \end{Bmatrix}$

The methods coincide at the limit of vanishing step-size when $\alpha = \sqrt{\frac{k}{m}}\Delta t \to 0$.

ACCURACY AND STABILITY

Numerical integration involves discretization error in each step and error accumulation may spoil the solution after certain number of steps. Crank-Nicolson does not reduce the amplitude but the phase error is clear from comparison of the exact and numerical solutions to a vibrating particle problem.





With multiple particles and various time-scales of vibrations, certain amount of numerical dumping is actually a desirable property of a numerical integration method!

Method	Iteration $i \in \{1, 2, \ldots\}$	Initial $i = 0$
DG	$\begin{bmatrix} \Delta t\mathbf{K} & -\frac{1}{2}\Delta t^2\mathbf{K} + \mathbf{M} \\ \frac{1}{2}\Delta t^2\mathbf{K} - \mathbf{M} & \Delta t\mathbf{M} - \frac{1}{6}\Delta t^3\mathbf{K} \end{bmatrix} \begin{Bmatrix} \mathbf{a} \\ \dot{\mathbf{a}} \end{Bmatrix}_i = \begin{bmatrix} \mathbf{0} & \mathbf{M} \\ -\mathbf{M} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \mathbf{a} \\ \dot{\mathbf{a}} \end{Bmatrix}_{i-1}$	$\begin{Bmatrix} \mathbf{a} \\ \dot{\mathbf{a}} \end{Bmatrix}_0 = \begin{Bmatrix} \mathbf{g} \\ \mathbf{h} \end{Bmatrix}$
CN	$\begin{bmatrix} \mathbf{I} & -\frac{\Delta t}{2}\mathbf{I} \\ \frac{\Delta t}{2}\mathbf{K} & \Delta t\mathbf{M} \end{bmatrix} \begin{Bmatrix} \mathbf{a} \\ \dot{\mathbf{a}} \end{Bmatrix}_i = \begin{bmatrix} \mathbf{I} & \frac{\Delta t}{2}\mathbf{I} \\ -\frac{\Delta t}{2}\mathbf{K} & \Delta t\mathbf{M} \end{bmatrix} \begin{Bmatrix} \mathbf{a} \\ \dot{\mathbf{a}} \end{Bmatrix}_{i-1}$	$\begin{Bmatrix} \mathbf{a} \\ \dot{\mathbf{a}} \end{Bmatrix}_0 = \begin{Bmatrix} \mathbf{g} \\ \mathbf{h} \end{Bmatrix}$

The proper step-size Δt depends on the largest eigenvalue of parameter $\alpha = \mathbf{M}^{-1}\mathbf{K}\Delta t^2$. The numerical damping of DG exceeds that of CN whereas the phase error of CN exceeds that of the DG method.

Derivation of the Crank-Nicolson method uses Taylor series with respect to time for displacement and velocity with the mean value approximation to the remainder

$$\mathbf{a}_i = \mathbf{a}_{i-1} + \Delta t \frac{\dot{\mathbf{a}}_{i-1} + \dot{\mathbf{a}}_i}{2}, \quad \dot{\mathbf{a}}_i = \dot{\mathbf{a}}_{i-1} + \Delta t \frac{\ddot{\mathbf{a}}_{i-1} + \ddot{\mathbf{a}}_i}{2}$$

and the differential equation written at the ends of the time interval

$$\mathbf{M}\ddot{\mathbf{a}}_{i-1} + \mathbf{K}\mathbf{a}_{i-1} - \mathbf{F}_{i-1} = 0, \quad \mathbf{M}\ddot{\mathbf{a}}_i + \mathbf{K}\mathbf{a}_i - \mathbf{F}_i = 0.$$

Solving for $\mathbf{a}_i$ and $\dot{\mathbf{a}}_i$ in terms of $\mathbf{a}_{i-1}$ and $\dot{\mathbf{a}}_{i-1}$ from the equations

$$\begin{bmatrix} \mathbf{I} & -\frac{\Delta t}{2}\mathbf{I} \\ \frac{\Delta t}{2}\mathbf{K} & \Delta t\mathbf{M} \end{bmatrix} \begin{Bmatrix} \mathbf{a} \\ \dot{\mathbf{a}} \end{Bmatrix}_i = \begin{bmatrix} \mathbf{I} & \frac{\Delta t}{2}\mathbf{I} \\ -\frac{\Delta t}{2}\mathbf{K} & \Delta t\mathbf{M} \end{bmatrix} \begin{Bmatrix} \mathbf{a} \\ \dot{\mathbf{a}} \end{Bmatrix}_{i-1} + \frac{\Delta t}{2}\left(\begin{Bmatrix} \mathbf{0} \\ \mathbf{F} \end{Bmatrix}_{i-1} + \begin{Bmatrix} \mathbf{0} \\ \mathbf{F} \end{Bmatrix}_i \right).$$

ONE-STEP METHOD

Taylor series with respect to time and the mean value approximation to the remainder (the number of terms or the approximation may differ from those below) give, e.g.,

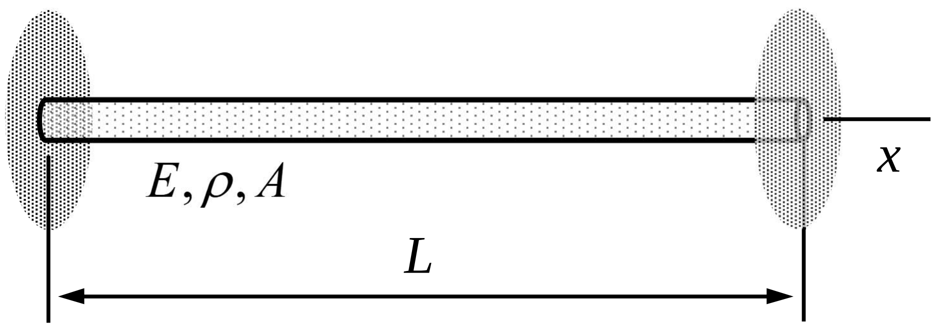
$$\mathbf{a}_i = \mathbf{a}_{i-1} + \Delta t \frac{\dot{\mathbf{a}}_{i-1} + \dot{\mathbf{a}}_i}{2} \quad \text{and} \quad \dot{\mathbf{a}}_i = \dot{\mathbf{a}}_{i-1} + \Delta t \frac{\ddot{\mathbf{a}}_{i-1} + \ddot{\mathbf{a}}_i}{2}$$

Differential equations written at the end points of the time interval contain the derivatives of the remainder terms (the equation may be differentiated more with respect to time

$$\mathbf{M}\ddot{\mathbf{a}}_{i-1} + \mathbf{K}\mathbf{a}_{i-1} - \mathbf{F}_{i-1} = 0 \quad \text{and} \quad \mathbf{M}\ddot{\mathbf{a}}_i + \mathbf{K}\mathbf{a}_i - \mathbf{F}_i = 0.$$

Solving the equations for $\mathbf{a}_i$ and $\dot{\mathbf{a}}_i$ in terms of $\mathbf{a}_{i-1}$ and $\dot{\mathbf{a}}_{i-1}$ gives the well-known Crank-Nicolson method. The same recipe applies with more terms in the Taylor series approximations to displacement and velocity.

EXAMPLE Finite Difference Method is applied to the bar problem shown using a regular grid with $i \in \{0,1,2,3\}$. Thereafter, Crank-Nicolson methods is applied to find the solution at the temporal grid $t_j = j\Delta t \quad j \in \{0,1,\ldots\}$. Derive the iteration formula giving the displacements and velocities of points of the spatial discretization for any initial displacement and velocities. Material properties E,ρ and cross-sectional area A are constants.



Answer $\dfrac{EA}{h^2}\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}\begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix} + \rho A \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{Bmatrix} \ddot{u}_1 \\ u_2 \end{Bmatrix} = 0$ where $h = \dfrac{L}{3}$

Use of the Finite Difference Method and 2:nd order central difference approximation on a regular grid with $i \in \{0,1,2,3\}$ gives the ordinary differential equations

$$\frac{EA}{h^2}\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}\begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix} + \rho A \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{Bmatrix} \ddot{u}_1 \\ u_2 \end{Bmatrix} = 0 \quad \text{where} \quad h = \frac{L}{3}$$

for the interior points 1 and 2. With notation

$$\mathbf{M} = \rho A \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \ \mathbf{K} = \frac{EA}{h^2}\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}, \ \mathbf{a} = \begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix}, \ \dot{\mathbf{a}} = \begin{Bmatrix} \dot{u}_1 \\ \dot{u}_2 \end{Bmatrix}, \ \mathbf{g} = \begin{Bmatrix} g_1 \\ g_2 \end{Bmatrix}, \ \text{and} \ \ \mathbf{h} = \begin{Bmatrix} h_1 \\ h_2 \end{Bmatrix}$$

the time-integration according to the Crank-Nicolson method follows from

$$\begin{bmatrix} \mathbf{I} & -\frac{\Delta t}{2}\mathbf{I} \\ \frac{\Delta t}{2}\mathbf{K} & \Delta t\mathbf{M} \end{bmatrix}\begin{Bmatrix} \mathbf{a} \\ \dot{\mathbf{a}} \end{Bmatrix}_i = \begin{bmatrix} \mathbf{I} & \frac{\Delta t}{2}\mathbf{I} \\ -\frac{\Delta t}{2}\mathbf{K} & \Delta t\mathbf{M} \end{bmatrix}\begin{Bmatrix} \mathbf{a} \\ \dot{\mathbf{a}} \end{Bmatrix}_{i-1} \quad \text{and} \quad \begin{Bmatrix} \mathbf{a} \\ \dot{\mathbf{a}} \end{Bmatrix}_0 = \begin{Bmatrix} \mathbf{g} \\ \mathbf{h} \end{Bmatrix}.$$