Finite Difference and Finite Element Methods

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COMPSCI 369 Computational Science

1. Finite Differences
2. Difference Equations
3. Finite Difference Methods: Euler FDMs
4. Finite Element Methods (FEM) [optional]

Learning outcomes:

- Be familiar with the finite difference models and methods (Euler FDMs)
- **Optional**: Runge-Kutta FDMs, more accurate FEMs

RECOMMENDED READING:

- M. T. Heath, Scientific Computing: An Introductory Survey. McGraw-Hill, 2002: Chapters 5, 8 – 11
- M. Shäfer, Computational Engineering - Introduction to Numerical Methods. Springer, 2006: Chapters 3, 5
- G. Strang, Computational Science and Engineering. Wellesley-Cambridge Press, 2007: Chapters 1.2, 3, 6

Let's Recall Differential Equations

Modern science and engineering assume our world is continuous and described by differential equations and integral equations

Example I: 1st-order differential equation $\frac{du(x)}{dx} = 2;\ u(0) = 0$

General solution:	$u(x) = 2x + A$
Boundary condition:	$u(0) = 0$ gives $A = 0$
Final solution:	$\rightarrow u(x) = 2x$

Unknown $u(x)$ is specified by a known **instant speed** of changes:

$$\frac{du(x)}{dx} = \lim_{\Delta x \to 0} \frac{u(x + \Delta x) - u(x)}{\Delta x}$$

Let's Recall Differential Equations, continued

Example II: 2nd-order DE $\frac{d^2u(x)}{dx^2} = 2;\ u(0) = u(1) = 0$

General solution:	$u(x) = x^2 + Ax + B$
Boundary conditions:	$u(0) = 0; u(1) = 0$ give $B = 0;\ A = 1$
Final solution:	$\rightarrow u(x) = x^2 - x$

Unknown $u(x)$ is specified by a known **instant acceleration** of changes:

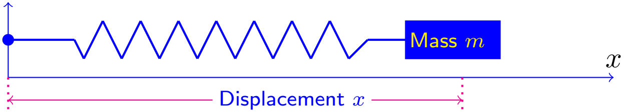
$$\frac{d^2u(x)}{dx^2} = \lim_{\Delta x \to 0} \frac{1}{\Delta x}\left(\frac{du(x+\Delta x)}{dx} - \frac{du(x)}{dx}\right)$$

$$= \lim_{\Delta x \to 0} \frac{1}{\Delta x}\left(\frac{u(x+2\Delta x)-u(x+\Delta x)}{\Delta x} - \frac{u(x+\Delta x)-u(x)}{\Delta x}\right)$$

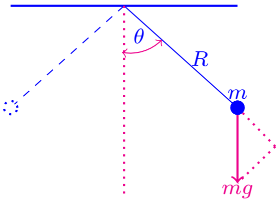
$$= \lim_{\Delta x \to 0} \frac{u(x+2\Delta x)-2u(x+\Delta x)+u(x)}{\Delta x^2}$$

Physical Oscillating Second-order Systems

- Non-damped mass on a spring: $-m\frac{d^2x(t)}{dt^2} = kx$
  - $x(t)$ – a displacement
  - k – a spring constant (the Hooke's law)
  - m – a mass



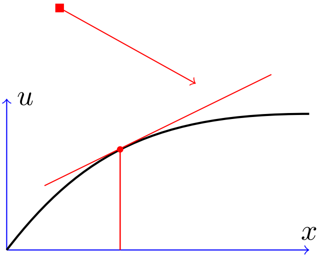
- Damped mass on a spring (γ – the friction constant): $-m\frac{d^2x(t)}{dt^2} = \gamma\frac{dx(t)}{dt} + kx$
- Pendulum: $-mR^2\frac{d^2\theta}{dt^2} = mgR\sin\theta$ $\Leftrightarrow -\frac{d^2\theta}{dt^2} = \frac{g}{R}\sin\theta$

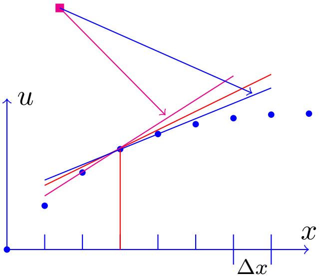


Differences Vs. Derivatives

Finite differences: natural approximations to **derivatives**

$$\frac{du(x)}{dx} = \lim_{\Delta x \to 0} \frac{u(x+\Delta x) - u(x)}{\Delta x} \Leftrightarrow \frac{\Delta u(x)}{\Delta x} \equiv \frac{u(x+\Delta x) - u(x)}{\Delta x}$$





Discrete step Δx can be small but **it does not tend to zero**!

Differences Vs. Derivatives

- Three possibilities for the finite difference:

		Test for $u(x) = x^2$
Forward difference	$\frac{u(x+h)-u(x)}{h}$	$\frac{(x+h)^2-x^2}{h} = 2x + h$
Backward difference	$\frac{u(x)-u(x-h)}{h}$	$\frac{x^2-(x-h)^2}{h} = 2x - h$
Centred difference	$\frac{u(x+h)-u(x-h)}{2h}$	$\frac{(x+h)^2-(x-h)^2}{2h} = 2x$

- Results of testing:
  - The centred difference gives the exact derivative $\frac{du(x)}{dx} = 2x$
  - The forward and the backward differences differ by h

Taylor Series Approximation

- Let $u(x)$ be an arbitrary infinitely differentiable function
  - In plain words, let all its derivatives exist:

$$\frac{d^n u(x)}{dx^n}; \quad 1 \le n \le \infty$$

- Given $u(x_0)$ and $\left.\frac{d^n u(x)}{dx^n}\right|_{x=x_0}$; $n = 1, 2, \ldots,$ at $x = x_0$, the value $u(x_0 + h)$ at $x = x_0 + h$ is represented by the Taylor's series of the values at $x = x_0$:

$$\begin{aligned} u(x_0 + h) &= u(x_0) + \sum_{n=1}^{\infty} \frac{h^n}{n!} \underbrace{\left.\frac{d^n (u(x))}{dx^n}\right|_{x=x_0}}_{\equiv u^{[n]}(x_0)} \\ &\equiv u(x_0) + \sum_{n=1}^{\infty} \frac{h^n}{n!} u^{[n]}(x_0) \end{aligned}$$

A Few Famous Taylor Series

- Exponential function $u(x) = e^x \Leftrightarrow e^0 = 1;\ \frac{de^x}{dx}\Big|_{x=0} = e^x\big|_{x=0} = 1:$

$$\Rightarrow u(0+h) \equiv e^h = 1 + h + \frac{h^2}{2} + \frac{h^3}{6} + \frac{h^4}{24} + \dots$$

- Polynomial ratio

$u(x) = \frac{1}{1+x^2} \Leftrightarrow u(0) = 1;\ \frac{du(x)}{dx}\Big|_{x=0} = \frac{-2x}{(1+x^2)^2}\Big|_{x=0} = 0;$

$\frac{d^2u(x)}{dx^2}\Big|_{x=0} = \left(-\frac{2}{(1+x^2)^2} + \frac{8x}{(1+x^2)^3}\right|_{x=0} = -2:$

$$u(0+h) \equiv \frac{1}{1+h^2} = 1-h^2+h^4-\dots \Rightarrow u(1) = \frac{1}{2} = 1 - 1 + 1 - 1 + \dots$$

- Trivial for any polynomial
  - $u(x) = x^3 - 2 \Leftrightarrow u(1) = 1;\ \frac{du(x)}{dx} = 3x^2;\ \frac{d^2u(x)}{dx^2} = 6x;\ \frac{d^3u(x)}{dx^3} = 6:$

$$\Rightarrow u(1+h) = -1 + 3h + 6\frac{h^2}{2} + 6\frac{h^3}{6} = -1 + 3h + 3h^2 + h^3$$

Accuracy of Finite Differences

Taylor series approximations:

$$
\begin{aligned}
u(x+h) &= u(x) + hu'(x) + \tfrac{1}{2}h^2u''(x) + \tfrac{1}{6}h^3u^{[3]}(x) + \dots \\
u(x-h) &= u(x) - hu'(x) + \tfrac{1}{2}h^2u''(x) - \tfrac{1}{6}h^3u^{[3]}(x) + \dots
\end{aligned}
$$

- The first-order accuracy $O(h)$ of the one-sided differences:

$$
\begin{aligned}
\tfrac{u(x+h)-u(x)}{h} &= u'(x) + \tfrac{1}{2}hu''(x) + \dots \\
\tfrac{u(x)-u(x-h)}{h} &= u'(x) + \tfrac{1}{2}hu''(x) + \dots
\end{aligned}
$$

- The second-order accuracy $O(h^2)$ of the centred differences:

$$
\frac{u(x+h)-u(x-h)}{2h} = u'(x) + \frac{1}{6}h^2u^{[3]}(x) + \dots
$$

Second Difference

The second difference approximation of the second derivative:

$$\frac{d^2u}{dx^2} \approx \frac{\Delta^2 u}{\Delta x^2} = \frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{\Delta x^2}$$

- The second order accuracy $O(h^2)$ due to the centred $\Delta^2 u$:

$$\frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{\Delta x^2} = u''(x) + \frac{1}{12}h^2 u^{[4]}(x) + \ldots$$

- Exact second derivatives $\frac{(x+h)^2 - 2x^2 + (x-h)^2}{h^2} = 2$ for $u(x) = x^2$ and $\frac{(x+h)^3 - 2x^3 + (x-h)^3}{h^2} = 6x$ for $u(x) = x^3$
- $O(h^2)$ accuracy $\frac{(x+h)^4 - 2x^4 + (x-h)^4}{h^2} = 12x^2 + h^2$ for $u(x) = x^4$ with the true second derivative $u''(x) = 12x^2$

Finite Difference Equations

The 2^{nd}-order **differential equation** $-\frac{d^2u(x)}{dx^2} = f(x)$

- Known **source** function $f(x)$
- Known boundary conditions, e.g. $u(0) = 0$ and $u(1) = 0$

Its discrete form – the 2^{nd}-order **finite difference equation**:

- Divide the interval $[0, 1]$ into equal pieces of length $h = \frac{1}{n+1}$ that meet at the points $x = h$, $x = 2h$, $\ldots$, $x = nh$:

- Approximate the goal values $u(h), \ldots, u(nh)$ at n discrete points $[h, 2h, \ldots, nh]$ inside the interval $[0, 1]$ with the values $u_1, \ldots, u_n$, respectively, using the finite difference $\frac{\Delta^2 u}{\Delta x^2}$:

$$u_0 - 2u_1 + u_2 = f_1 \equiv f(h); \quad u_1 - 2u_2 + u_3 = f_2 \equiv f(2h);$$
$$\ldots \qquad u_{n-1} - 2u_n + u_{n+1} = f_n \equiv f(nh)$$

Finite Difference Equations: Matrix-Vector Form

For the n unknowns $u_1, u_2, \ldots, u_n$ and the boundary conditions $u_0 = u_{n+1} = 0$, the differential operator $\frac{d^2}{dx^2}$ is replaced with the $n \times (n+2)$ matrix:

$$-\frac{1}{h^2}\begin{bmatrix} 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & 1 & -2 & 1 & \\ & & & & 1 & -2 & 1 \end{bmatrix}\begin{bmatrix} u_0 = 0 \\ u_1 \\ \vdots \\ u_n \\ u_{n+1} = 0 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{n-1} \\ f_n \end{bmatrix}$$

where the source values are specified as $f_i = f(ih)$

- For the special case $\frac{d^2u}{dx^2} = 1$ with the above boundary conditions, the finite differences give an exact match between $u(ih)$ and u_i

Example with the Constant Source $f(x) = 1$

- **Differential equation**: $-\frac{d^2u}{dx^2} = 1$ with $u(0) = u(1) = 0$
  - Complete solution $u_{\text{complete}} = u_{\text{part}} + u_{\text{null}}$: a particular one for $u'' = 1$ plus the nullspace one for $u'' = 0$
  - Particular solution: $-\frac{d^2u}{dx^2} = 1$ is solved by $u_{\text{part}} = -\frac{x^2}{2}$
  - Nullspace solution: $-\frac{d^2u}{dx^2} = 0$ is solved by $u_{\text{null}} = Cx + D$
  - $u(x) = \frac{x^2}{2} + Cx + D \Rightarrow$ From the boundary conditions:
    - $u(0) = D = 0$
    - $u(1) = -\frac{1}{2} + C + D = 0 \rightarrow C = -\frac{1}{2} \Rightarrow$
    - $u(x) = \frac{x - x^2}{2}$
- **Difference equation**: $\frac{-u_{i-1} + 2u_i - u_{i+1}}{h^2} = 1$ with $u_0 = u_{n+1} = 0$
  - **(!)** Just the same parabolic solution: $u_i = \frac{ih - i^2h^2}{2}$
  - However such a perfect agreement between the discrete u_i and the exact continuous $u(ih)$ is very unusual

Another Example: Free End Boundary Condition (optional)

Free end condition: zero slope $u'(0) = 0$ at $x = 0$ and $u(1) = 0$

- **Differential equation**: $-\frac{d^2u}{dx^2} = 1$ with $\frac{du}{dx}(0) = u(1) = 0$
  - The complete solution: $u(x) = -\frac{x^2}{2} + Cx + D = \frac{1-x^2}{2}$
  - Boundary conditions:
    $u'(0) = C = 0; u(1) = -0.5 + C + D = 0 \rightarrow D = 0.5$
- **Difference equation**: $\frac{-u_{i-1}+2u_i-u_{i+1}}{h^2} = 1$ with $\frac{u_1-u_0}{h} = 0$ and $u_{n+1} = 0$

$$-\frac{1}{h^2}\underbrace{\begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & 1 \\ & & & -1 & 2 \end{bmatrix}}_{\mathbf{T}_n}\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{bmatrix}$$

Free End Boundary Condition, continued

$$\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = h^2 \underbrace{\begin{bmatrix} n & n-1 & n-2 & \dots & 1 \\ n-1 & n-1 & n-2 & \dots & 1 \\ n-2 & n-2 & n-2 & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & 1 \\ 1 & 1 & 1 & \dots & 1 \end{bmatrix}}_{\mathbf{T}_n^{-1}} \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{bmatrix}$$

Discrete solution: $u_i = h^2 \frac{(n+i)(n+1-i)}{2}$

- Error w.r.t. the exact solution:

$$\begin{aligned} u(ih) - u_i &\equiv u\left(\frac{i}{n+1}\right) - u_i = \frac{1}{2}\left(1 - \frac{i^2}{(n+1)^2}\right) - \frac{1}{2}\frac{(n+i)(n+1-i)}{(n+1)^2} \\ &= \frac{1}{2}\frac{n+1-i}{(n+1)^2} = \frac{1}{2}\left(\frac{1}{n+1} - \frac{i}{(n+1)^2}\right) \Rightarrow O(h) \end{aligned}$$

Free End Boundary Condition, continued

- Therefore, the one-sided boundary conditions change the matrix and may result in $O(h)$ error
- A more accurate difference equation can be constructed by centring the boundary conditions
- Centred difference equation will have 2^{nd}-order errors $O(h^2)$
- Previous and similar differential and difference equations can be met in many practical problems
    - Simple physical examples of oscillators (see Slide 5):
        - a non-damped mass on a spring
        - a damped mass on a spring
        - a pendulum

Stiff Differential Equations

Example: $\frac{d}{dt}\begin{bmatrix} v \\ w \end{bmatrix} = \overbrace{\begin{bmatrix} -50 & 49 \\ 49 & -50 \end{bmatrix}}^{\mathbf{A}} \begin{bmatrix} v \\ w \end{bmatrix}; \begin{bmatrix} v(0) \\ w(0) \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$

Solution: $v(t) = e^{-t} + e^{-99t}$ and $w(t) = e^{-t} - e^{-99t}$

- Time scales differ by a factor of 99 (the condition number of $\mathbf{A}$)
- Solution decays at the slow time scale of e^{-t}, but computing e^{-99t} may require a very small step Δt for stability
- Thus, Δt is controlled by the fast decaying component, and this is really counterproductive!

Stiffness comes with any problem involving very different time scales (chemical kinetics, control theory, circuit simulations, etc.)

Forward and Backward Euler Methods (optional)

- Differential equation $\frac{du(t)}{dt} = f(u,t)$; an initial value $u(0)$
  - The rate of change u' is determined by the current state u at any moment t
- Forward Euler:

$$\frac{u_{n+1} - u_n}{\Delta t} = f(u_n, t_n) \Rightarrow u_{n+1} = u_n + \Delta t \cdot f_n$$

- Backward Euler:

$$\frac{u_{n+1} - u_n}{\Delta t} = f(u_{n+1}, t_{n+1}) \Rightarrow u_{n+1} - \Delta t \cdot f_{n+1} = u_n$$

  - Implicit method: if f is linear in u, a linear system is solved at each step

Forward and Backward Euler Methods, continued

Example: Linear differential equation $u' = au$ (i.e. $\frac{du(t)}{dt} = au$);

$u(0) = u_0 > 0$, with the exact solution: $u(t) = e^{at}u(0) \equiv u_0 e^{at}$

Generally, a is a complex number: $a = (\mathrm{Re}\, a) + (\mathrm{Im}\, a)\sqrt{-1}$

- **Forward Euler**:
  one step $u_{n+1} = (1 + a\Delta t)u_n \;\rightarrow\; u_n = (1 + a\Delta t)^n u_0$
  - Convergence: $(1 + a\Delta t)^{T/\Delta t} \rightarrow e^{aT}$ as $\Delta t \rightarrow 0$
  - Sharp **instability** border $1 + a\Delta t = -1$, i.e. for $a = -2/\Delta t$
- **Backward Euler**:
  one step $(1 - a\Delta t)u_{n+1} = u_n \;\rightarrow\; u_n = (1 - a\Delta t)^{-n} u_0$
  - Convergence: $(1 - a\Delta t)^{-1} = 1 + a\Delta t +$ *higher order terms*, so that $(1 - a\Delta t)^{-T/\Delta t} \rightarrow e^{aT}$ as $\Delta t \rightarrow 0$
  - Stability whenever $u' = au$ is stable (i.e. for a having the negative real part: $\mathrm{Re}\, a < 0$)

Forward and Backward Euler Methods, continued

Since forward and backward differences are *first order accurate*, the errors from both methods are $O(\Delta t)$

Second-order methods:

- Formal notation: $f_n = f(u_n, t_n)$ and $f_{n+1} = f(u_{n+1}, t_{n+1})$
- Crank-Nicolson:

$$\frac{u_{n+1} - u_n}{\Delta t} = \frac{f_{n+1} + f_n}{2} \Rightarrow u_{n+1} = \frac{1 + \frac{1}{2}a\Delta t}{1 - \frac{1}{2}a\Delta t} u_n$$

  - Stable even for stiff equations, when $a \ll 0$

Forward and Backward Euler Methods, continued

Second-order methods:

- Explicit forward Euler:

$$\frac{u_{n+1} - u_n}{\Delta t} = \frac{3f_n - f_{n-1}}{2}$$

  - Stable if Δt is small enough: $-a\Delta t \leq 1$ if a is real
  - But explicit systems always impose a limit on Δt

- Implicit backward difference:

$$\frac{3u_{n+1} - 4u_n + u_{n-1}}{2\Delta t} = f_{n+1}$$

  - More stable and accurate than the Crank-Nicolson method (trapezoidal rule)

Explicit and Implicit Multistep Methods (optional)

With p earlier values of u_n, the accuracy is increased to order p

$$\begin{aligned}
\nabla u &= u(t) - u(t-\Delta t) \\
\nabla^2 u &= u(t) - 2u(t-\Delta t) + u(t-2\Delta t) \\
\nabla^3 u &= u(t) - 3u(t-\Delta t) + 3u(t-2\Delta t) - u(t-3\Delta t) \\
\dots \\
\nabla^p u &= u(t) - pt(y-\Delta t) + \ldots + (-1)^p u(t-p\Delta t)
\end{aligned}$$

- Backward differences:
$$\left(\nabla + \frac{1}{2}\nabla^2 + \ldots + \frac{1}{p}\nabla^p\right) u_{n+1} = \Delta t \cdot f(u_{n+1}, t_{n+1})$$
  - Backward Euler method: $p = 1$
  - Implicit backward difference method: $p = 2$

Explicit and Implicit Multistep Methods, continued

An alternative: using older values of $f(u_n, t_n)$ instead of u_n

- Explicit forward Euler methods:

$$u_{n+1} - u_n = \Delta t \cdot (b_1 f_n + \ldots + b_p f_{n-p+1})$$

order of accuracy	b_1	b_2	b_3	b_4	limit on $-a\Delta t$ for stability
$p=1$	1				2
$p=2$	3/2	-1/2			1
$p=3$	23/12	-16/12	5/12		6/11
$p=4$	55/24	-59/24	37/24	-9/24	3/10

- The like implicit methods are even more stable and accurate

Runge-Kutta Methods (optional)

- Highly competitive and self-starting if evaluations of $f(u,t)$ are not too expensive
- **Compound** 1-step methods, using Euler's $u_n + \Delta t f_n$ **inside the function** f
- **Simplified RKM**:

$$\frac{u_{n+1} - u_n}{\Delta t} = \frac{1}{2}\left[f_n + \underbrace{f(u_n + \Delta t f_n, t_{n+1})}_{\text{compounding of } f} \right]$$

Simplified Runge-Kutta Method (optional)

- 2^{nd}-order accuracy
- An example for $u' = au$:

$$\begin{aligned} u_{n+1} &= u_n + \tfrac{1}{2}\Delta t[au_n + a(u_n + \Delta t a u_n)] \\ &= \underbrace{\left(1 + a\Delta t + \frac{1}{2}a^2\Delta t^2\right)}_{\text{Growth factor } G} u_n \end{aligned}$$

- This growth factor G reproduces the exact $e^{a\Delta t}$ through the third term $\frac{1}{2}a^2(\Delta t)^2$ of the Taylor's series

Higher-order Runge-Kutta Method (optional)

- **Fourth-order RKM**: $\frac{u_{n+1}-u_n}{\Delta t} = \frac{1}{3}(k_1 + 2k_2 + 2k_3 + k_4)$ where

$$k_1 = \frac{1}{2}f(u_n, t_n) \qquad k_3 = \frac{1}{2}f\left(u_n + \Delta t k_2, t_{n+1/2}\right)$$

$$k_2 = \frac{1}{2}f\left(u_n + \Delta t k_1, t_{n+1/2}\right) \qquad k_4 = \frac{1}{2}f\left(u_n + 2\Delta t k_3, t_{n+1}\right)$$

  - This 1-step method needs no special starting instructions
  - It is simple to change Δt during computations
  - The growth factor reproduces $e^{a\Delta t}$ through the fifth term $\frac{1}{24}a^4(\Delta t)^4$ of the Taylor's series
  - **Among highly accurate methods, RKM is especially easy to code and run – probably the easiest there is!**
  - The stability threshold is $-a\Delta t < 2.78$

Finite Element Methods (FEM) [optional]

Finite difference methods (FDM) approximate the differential equation

(+) Very easy implementation

(−) Low accuracy between grid points

Finite element methods (FEM) approximate directly the solution of the differential equation

(+) Easy handling of complex geometry and boundaries of a problem domain

(±) Usually, more accurate than FDM but this depends on a problem

- Unknown solution $u(x)$ as a combination of n basis functions $\phi(x)$:
$$u(x) = u_1\phi_1(x) + \ldots + u_n\phi_n(x)$$
- FDM are special cases of the FEM with specific basis functions

Finite Element Methods: Weak Form

- **Weak** (or variational) form of the differential equation $-u''(x) = f(x)$ in $[0, 1]$ with $u(0) = u(1) = 0$:
  - For any smooth function $\nu(x)$ satisfying the boundary conditions $\nu(0) = \nu(1) = 0$:

$$\int_0^1 f(x)\nu(x)dx = -\int_0^1 u''(x)\nu(x)dx = \int_0^1 u'(x)\nu'(x)dx$$

Recall the calculus: Integration by parts

$$\int_a^b y(s)z'(s)ds = y(s)z(s)|_a^b - \int_a^b y'(s)z(s)ds$$

Galerkin's FEM: $-u'' = f$ in the discrete weak form

Discretisation of $\nu(x)$ with n "test functions" $\nu_1(x), \ldots, \nu_n(x)$

- The weak form gives one equation for each $\nu_j(x)$ involving numerical coefficients $u_1, \ldots, u_n$:

$$\int_0^1 \left(\sum_{i=1}^{n} u_i \frac{d\phi_i(x)}{dx} \right) \frac{d\nu_j(x)}{dx} dx = \int_0^1 f(x)\nu_j(x)dx; \; j = 1, \ldots, n$$

$$\Rightarrow \; \mathbf{K}\mathbf{u} = \mathbf{f},$$

that is, $\sum_{i=1}^{n} K_{ij} u_i = f_j; \; j = 1, \ldots, n$, where

$$K_{ij} = \int_0^1 \left(\frac{d\phi_i(x)}{dx} \frac{d\nu_j(x)}{dx} \right) dx \text{ and } f_j = \int_0^1 f(x)\nu_j(x)dx$$

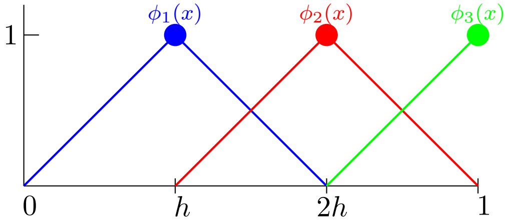
Galerkin's FEM: $-u'' = f$ (cont.)

- Mostly, the test functions ν_i's are the same as the basis functions ϕ_i's for $u(x)$
- Then the **stiffness matrix $\mathbf{K}$** is symmetric and positive definite
    - Integrals of products of $\phi_i(x)$ and $\nu_i(x)$ giving the matrix components K_{ij} should be finite ($-\infty < K_{ij} < \infty$)
        - So step functions are not allowed as the basis and test functions!
        - Derivative of a step-function is the delta-function δ, and the squared delta-function δ^2 has an infinite integral
    - Linear hat functions (having step functions as their derivatives) can be used as the basis and test functions

Linear Finite Elements: Hat Functions

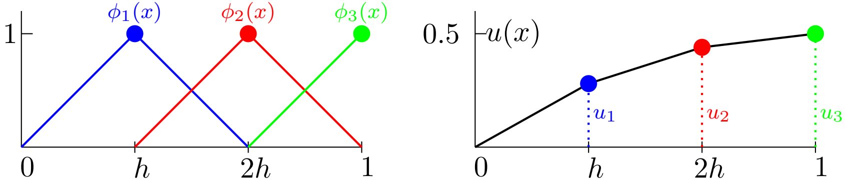
$$h = \frac{1}{3};\ u(x) = u_1\phi_1(x) + u_2\phi_2(x) + u_3\phi_3(x)$$

Basis and test functions $\phi_i(x) = \nu_i(x)$; $i = 1, 2, 3$:



	$\phi_1(x)$	$\phi_2(x)$	$\phi_3(x)$
$0 \le x \le \frac{1}{3}$	$3x$	0	0
$\frac{1}{3} \le x \le \frac{2}{3}$	$2 - 3x$	$3x - 1$	0
$\frac{2}{3} \le x \le 1$	0	$3 - 3x$	$3x - 2$

Linear Finite Elements: An Example with Hat Functions



Piecewise-linear function $u(x) = u_1\phi_1(x) + u_2\phi_2(x) + u_3\phi_3(x)$

- **Differential equation**: $-u'' = 1$ (i.e. $f(x) = 1$)
  Free-end border conditions $u(0) = 0$; $u'(0) = 1$
  - **Complete solution** of this differential eqution:
    $u(x) = A + Bx - \frac{x^2}{2}$ (nullspace + a particular solution);
    $A = 0$ and $B = 1$ (from the border conditions) $\Rightarrow u(x) = x - \frac{x^2}{2}$
  - **Test functions**:
    ν_i: hats ϕ_1 and ϕ_2 and one half-hat ϕ_3; $h = \frac{1}{3}$

FEM Example with Hat Functions (cont.)

Stiffness matrix:

$$\mathbf{K} = \left[K_{ij} = \int_0^1 \frac{d\phi_i(x)}{dx} \frac{d\phi_j(x)}{dx} dx \right]_{i,j=1}^{3} = \begin{bmatrix} 6 & -3 & 0 \\ -3 & 6 & -3 \\ 0 & -3 & 3 \end{bmatrix}$$

	$\frac{d\phi_1(x)}{dx}$	$\frac{d\phi_2(x)}{dx}$	$\frac{d\phi_3(x)}{dx}$
$0 \leq x \leq \frac{1}{3}$	3	0	0
$\frac{1}{3} \leq x \leq \frac{2}{3}$	-3	3	0
$\frac{2}{3} \leq x \leq 1$	0	-3	3

E.g.

$$K_{11} = \int_0^1 \left(\frac{d\phi_1(x)}{dx} \right)^2 dx = 9 \cdot \tfrac{1}{3} + 9 \cdot \tfrac{1}{3} + 0 \cdot \tfrac{1}{3} = 6$$

$$K_{12} = \int_0^1 \frac{d\phi_1(x)}{dx} \frac{d\phi_2(x)}{dx} dx = 0 \cdot \tfrac{1}{3} - 9 \cdot \tfrac{1}{3} + 0 \cdot \tfrac{1}{3} = -3$$

FEM Example with Hat Functions (cont.)

Vector f $= [f_1, f_2, f_3]^\mathsf{T} = \left[\frac{1}{3}, \frac{1}{3}, \frac{1}{6}\right]^\mathsf{T}$:

$$
\begin{aligned}
f_1 = \int_0^1 \phi_1(x)dx &= \int_0^{1/3} 3x\,dx + \int_{1/3}^{2/3} (2-3x)dx \\
&= \frac{3x^2}{2}\Big|_0^{1/3} + \left(2x - \frac{3x^2}{2}\right)\Big|_{1/3}^{2/3} &&= \frac{1}{6} + \frac{1}{6} = \frac{1}{3} \\
f_2 = \int_0^1 \phi_2(x)dx &= \int_{1/3}^{2/3} (3x-1)dx + \int_{2/3}^{1} (3-3x)dx \\
&= \left(\frac{3x^2}{2} - x\right)\Big|_{1/3}^{2/3} + \left(3x - \frac{3x^2}{2}\right)\Big|_{2/3}^{1} &&= \frac{1}{6} + \frac{1}{6} = \frac{1}{3} \\
f_3 = \int_0^1 \phi_3(x)dx &= \int_{2/3}^{1} (3x-2)dx \\
&= \left(\frac{3x^2}{2} - 2x\right)\Big|_{2/3}^{1} &&= \frac{1}{6}
\end{aligned}
$$

FEM Example with Hat Functions (cont.)

Solving the finite element equation $\mathbf{K}\mathbf{u} = \mathbf{f}$ for the mesh values in $\mathbf{u}$:

$$\underbrace{\begin{bmatrix} 6 & -3 & 0 \\ -3 & 6 & -3 \\ 0 & -3 & 3 \end{bmatrix}}_{\mathbf{K}} \underbrace{\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}}_{\mathbf{u}} = \underbrace{\begin{bmatrix} 1/3 \\ 1/3 \\ 1/6 \end{bmatrix}}_{\mathbf{f}}$$

$$\Rightarrow \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \underbrace{\begin{bmatrix} 5/18 \\ 4/9 \\ 1/2 \end{bmatrix}}_{\mathbf{K}^{-1}\mathbf{f}} \Leftrightarrow u(x) = x - \frac{x^2}{2} = \begin{cases} 5/18 & x = 1/3 \\ 4/9 & x = 2/3 \\ 1/2 & x = 1 \end{cases}$$

- All three values u_1, u_2, u_3 agree exactly with the true solution of the differential equation $u(x) = x - \frac{x^2}{2}$ at the mesh points
- Values u_i by the finite differences were not exact for this equation

Finite Element Methods Vs. Finite Differences

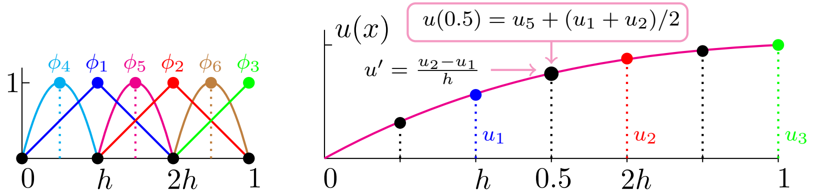
FEM: two- and three-dimensional meshes of arbitrary geometry, compared to the inflexibility of a finite difference grid

- Using numerical integration for $\mathbf{K}$ and $\mathbf{f}$, FEM allows for any functions $f(x)$ and $c(x)$ in solving the differential equation
$$\frac{d}{dx}\left(c(x)\frac{du(x)}{dx}\right) = f(x)$$
- Linear finite elements:
  - 2nd-order accuracy $O(h^2)$ in $u(x)$ and
  - 1st-order accuracy $O(h)$ in $\frac{du(x)}{dx}$
- Better accuracy – the higher-degree finite elements
  - E.g. piecewise cubic polynomials with continuous slopes
  - Adding to the hat functions the bubble functions: quadratic parabolas staying inside each mesh interval

More Accurate Finite Elements (optional)

Hat + bubble functions → piecewise linear slope $u'(x)$:

$$u(x) = u_1\phi_1(x) + u_2\phi_2(x) + u_3\phi_3(x) + u_4\phi_4(x) + u_5\phi_5(x) + u_6\phi_6(x)$$



- Expected accuracy: 3rd-order $O(h^3)$ in $u(x)$ and
  2nd-order $O(h^2)$ in $u'(x)$
- This higher accuracy – without a very fine mesh required by only linear elements!

Numerical Linear Algebra

- Applied Mathematics (AM) Vs. Computational Science (CS):
  - (AM) Stating a problem and building an equation to describe it
  - (CS) Solving that equation using mostly numerical methods
- Numerical linear algebra represents this "build up, break down" process in its clearest form, with matrix models like $\mathbf{Ku} = \mathbf{f}$
- Crucial properties of $\mathbf{K}$:
  - symmetric or not
  - sparse or not
  - banded or not
  - well conditioned or not
- Often the computations break $\mathbf{K}$ into simpler pieces

The algorithm becomes clearest when it is seen as a factorisation into:
triangular matrices or
orthogonal matrices or
very sparse matrices