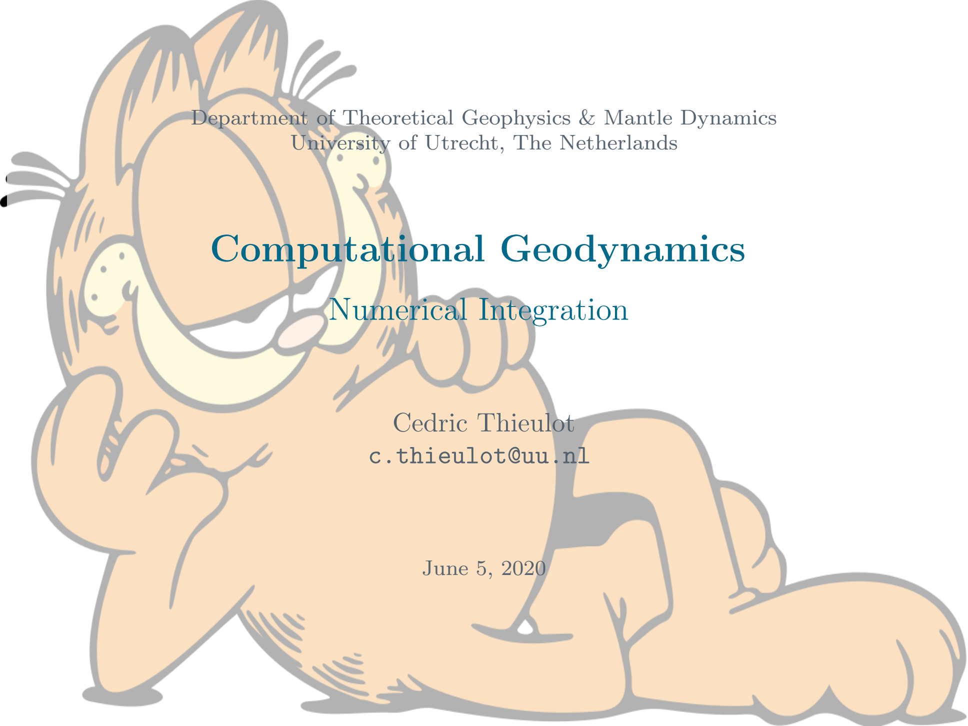

Department of Theoretical Geophysics & Mantle Dynamics
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# Computational Geodynamics

## Numerical Integration

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# Numerical integration
## Introduction



- The basic problem in numerical integration is to compute an approximate solution to a definite integral

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to a given degree of accuracy.

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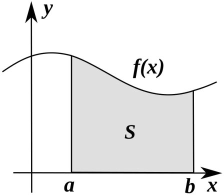
  to a given degree of accuracy.
- If $f(x)$ is a smooth function, and the domain of integration is bounded, there are many methods for approximating the integral to the desired precision.



# Numerical integration
## Reasons



There are several reasons for carrying out numerical integration.

- The integrand f(x) may be known only at certain points, such as obtained by sampling. Some embedded systems and other computer applications may need numerical integration for this reason.

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- A formula for the integrand may be known, but it may be difficult or impossible to find an antiderivative that is an elementary function. An example of such an integrand is $f(x) = exp(-x^2)$, the antiderivative of which (the error function, times a constant) cannot be written in elementary form.

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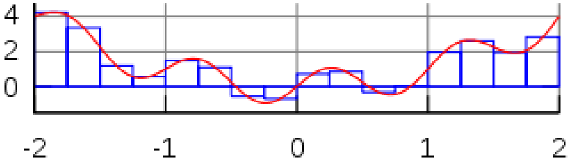
- It may be possible to find an antiderivative symbolically, but it may be easier to compute a numerical approximation than to compute the antiderivative. That may be the case if the antiderivative is given as an infinite series or product, or if its evaluation requires a special function that is not available.

The simplest method of this type is to let the interpolating function be a constant function (a polynomial of degree zero) that passes through the point ((a+b)/2, f((a+b)/2)).
This is called the midpoint rule or rectangle rule.

$$\int_a^b f(x)dx \simeq (b-a)f(\frac{a+b}{2})$$

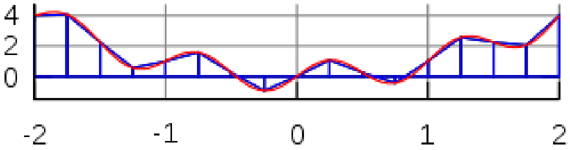


If we divide the interval into 4 subintervals:

$$
\begin{aligned}
& \int_0^1 f(x)dx \\
= \quad & \int_0^{0.25} f(x)dx + \int_{0.25}^{0.5} f(x)dx + \int_{0.5}^{0.75} f(x)dx + \int_{0.75}^{1} f(x)dx \\
\simeq \quad & 0.25 f(0.125) + 0.25 f(0.375) + 0.25 f(0.625) + 0.25 f(0.875)
\end{aligned}
$$

The interpolating function may be a straight line (an affine function, i.e. a polynomial of degree 1) passing through the points $(a, f(a))$ and $(b, f(b))$.
This is called the trapezoidal rule.

$$\int_a^b f(x)dx \simeq (b-a)\frac{f(a)+f(b)}{2}$$



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= \quad & 0.25\frac{f(0)+f(0.25)}{2} + 0.25\frac{f(0.25)+f(0.5)}{2} + \\
& 0.25\frac{f(0.5)+f(0.75)}{2} + 0.25\frac{f(0.75)+f(1)}{2} \\
= \quad & 0.25\left(\frac{f(0)}{2} + f(0.25) + f(0.5) + f(0.75) + \frac{f(1)}{2}\right)
\end{aligned}
$$

# Numerical integration



For either one of these rules, we can make a more accurate approximation by breaking up the interval $[a, b]$ into some number $n$ of subintervals, computing an approximation for each subinterval, then adding up all the results.
The midpoint rule can be stated as

$$\int_a^b f(x)dx \simeq h \sum_{k=0}^{n-1} f(a + (k + 1/2)h) \qquad h = (b-a)/n$$

where the subintervals are $[kh, (k+1)h]$, $k = 0, 1, \dots, n-1$.
The composite trapezoidal rule can be stated as

$$\int_a^b f(x)dx \simeq h \left( \frac{f(a)}{2} + \sum_{k=1}^{n-1} f(a + kh) + \frac{f(b)}{2} \right)$$

# Numerical integration
in 1D



Exercise 1: Write a program which uses the midpoint rule to compute (subdivide the interval in $n$ subintervals)

$$I = \int_0^{\pi/2} f(x)\,dx \qquad f(x) = x \qquad \text{and} \qquad f(x) = cos(x)$$

Compute and plot the (absolute) error between the measured $I_n$ and the analytical value $I$ as a function of the subinterval size $h$.

Exercise 2: Same exercise as above but with the trapezoidal rule.

Which method is the most accurate?

Bonus: Repeat Ex.1 with $I = \int_1^3 \int_2^4 (x^2 y^3 + xy + 1) dxdy$

# Numerical integration



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# Numerical integration



- Interpolation with polynomials evaluated at equally spaced points in $[a, b]$ yields the Newton–Cotes formulas, of which the rectangle rule and the trapezoidal rule are examples.
- If we allow the intervals between interpolation points to vary, we find another group of quadrature formulas, such as the Gaussian quadrature formulas.
- A Gaussian quadrature rule is typically more accurate than a Newton–Cotes rule, which requires the same number of function evaluations, if the integrand is smooth (i.e., if it is sufficiently differentiable).

# Numerical integration
## Gaussian quadrature



- In numerical analysis, a quadrature rule is an approximation of the definite integral of a function, usually stated as a weighted sum of function values at specified points within the domain of integration.

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- An $n-$point Gaussian quadrature rule, named after Carl Friedrich Gauss, is a quadrature rule constructed to yield an exact result for polynomials of degree $2n-1$ or less by a suitable choice of the points $x_i$ and weights $w_i$ for $i=1,\dots,n$.

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- The domain of integration for such a rule is conventionally taken as $[-1, 1]$, so the rule is stated as

$$\int_{-1}^{+1} f(x) dx = \sum_{i_q=1}^{n} w_{i_q} f(x_{i_q})$$


Johann Carl Friedrich Gauss (30 April 1777 – 23 February 1855)

# Numerical integration
## Gaussian quadrature



- Gaussian quadrature will only produce good results if the function $f(x)$ is well approximated by a polynomial function within the range $[-1, 1]$.

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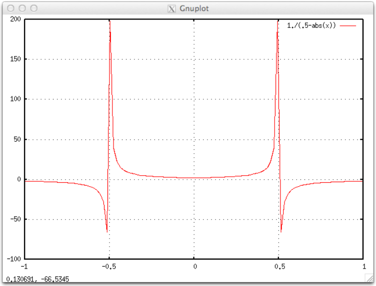
- The method is not, for example, suitable for functions with singularities.

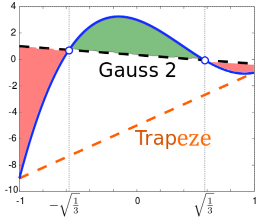


## Gauss-Legendre points and their weights

| Number of points, $n$ | Points, $x_i$ | Weights, $w_i$ |
|---|---|---|
| 1 | 0 | 2 |
| 2 | $\pm\sqrt{\frac{1}{3}}$ | 1 |
| 3 | 0 | $\frac{8}{9}$ |
| | $\pm\sqrt{\frac{3}{5}}$ | $\frac{5}{9}$ |
| 4 | $\pm\sqrt{\frac{3}{7}-\frac{2}{7}\sqrt{\frac{6}{5}}}$ | $\frac{18+\sqrt{30}}{36}$ |
| | $\pm\sqrt{\frac{3}{7}+\frac{2}{7}\sqrt{\frac{6}{5}}}$ | $\frac{18-\sqrt{30}}{36}$ |
| 5 | 0 | $\frac{128}{225}$ |
| | $\pm\frac{1}{3}\sqrt{5-2\sqrt{\frac{10}{7}}}$ | $\frac{322+13\sqrt{70}}{900}$ |
| | $\pm\frac{1}{3}\sqrt{5+2\sqrt{\frac{10}{7}}}$ | $\frac{322-13\sqrt{70}}{900}$ |

$x_i$ is the $i$-th root of the Legendre polynomial $P_n(x)$

Comparison between 2-point Gaussian and trapezoidal quadrature.




Blue line: polynomial $y(x) = 7x^3 - 8x^2 - 3x + 3$ with $\int\limits_{-1}^{+1} y(x)dx = 2/3$

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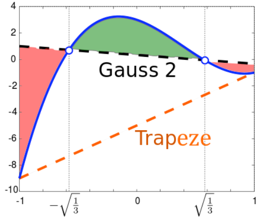


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The trapezoidal rule returns the integral of the orange dashed line, equal to $y(-1) + y(1) = -10$

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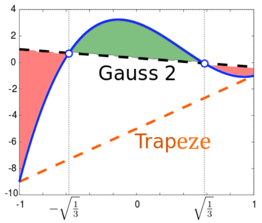


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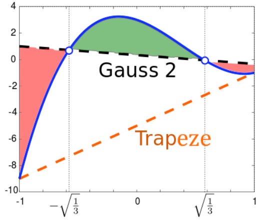


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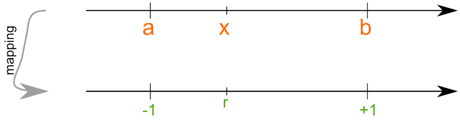
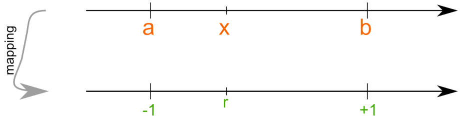
Such a result is exact, since the green region has the same area as the sum of the red regions.




- An integral over $[a, b]$ must be changed into an integral over $[-1, 1]$ before applying the Gaussian quadrature rule.

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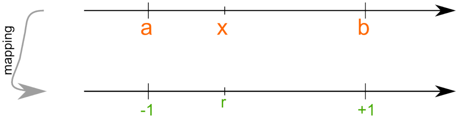
- This change of interval can be done in the following way:

$$r = \frac{2}{b-a}(x-a) - 1 \qquad x = \frac{b-a}{2}(1+r) + a \qquad dx = \frac{b-a}{2}dr$$

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$$\int_a^b f(x)dx = \frac{b-a}{2} \int_{-1}^{+1} f(r)dr \simeq \frac{b-a}{2} \sum_{i_q=1}^{n} w_{i_q} f(r_{i_q})$$

# Numerical integration
## Gaussian quadrature, example 1



For simplicity, $a = -1$, $b = +1$.
Let us take $f(x) = \pi$

$$I = \int_{-1}^{+1} f(x)dx = \pi \int_{-1}^{+1} dx = 2\pi$$

For simplicity, $a=-1$, $b=+1$.
Let us take $f(x)=\pi$

$$I=\int_{-1}^{+1} f(x)dx = \pi\int_{-1}^{+1} dx = 2\pi$$

$$I_{gq}=\int_{-1}^{+1} f(x)dx = \sum_{i_q=1}^{n_q} w_{i_q} f(x_{i_q}) = \sum_{i_q=1}^{n_q} w_{i_q}\pi = \pi\sum_{i_q=1}^{n_q} w_{i_q} = 2\pi$$

since $\sum_{i_q} w_{i_q} = 2$ !

# Numerical integration
## Gaussian quadrature, example 2



Let us now take $f(x) = mx + p$

$$I = \int_{-1}^{+1} f(x)dx = \int_{-1}^{+1} (mx+p)dx = \left[\frac{1}{2}mx^2 + px + C\right]_{-1}^{+1} = 2p$$

# Numerical integration
## Gaussian quadrature, example 2



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$$\begin{aligned} I_{gq} &= \int_{-1}^{+1} f(x)dx = \sum_{i_q=1}^{n_q} w_{i_q} f(x_{i_q}) = \sum_{i_q=1}^{n_q} w_{i_q} (m x_{i_q} + p) \\ &= m \underbrace{\sum_{i_q=1}^{n_q} w_{i_q} x_{i_q}}_{=0} + p \underbrace{\sum_{i_q=1}^{n_q} w_{i_q}}_{=2} = 2p \end{aligned}$$

since the quadrature points are symmetric w.r.t. to zero on the x-axis.

Let us take $f(x) = x^2$

$$I = \int_{-1}^{+1} f(x)dx = \int_{-1}^{+1} x^2 dx = \left[\frac{1}{3}x^3\right]_{-1}^{+1} = \frac{2}{3}$$

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$$I_{gq} = \int_{-1}^{+1} f(x)dx = \sum_{i_q=1}^{n_q} w_{i_q} f(x_{i_q}) = \sum_{i_q=1}^{n_q} w_{i_q} x_{i_q}^2$$

- $nq = 1$: $x_{iq}^{(1)} = 0$, $w_{i_q} = 2$. $I_{gq} = 0$

Let us take $f(x) = x^2$

$$I = \int_{-1}^{+1} f(x)dx = \int_{-1}^{+1} x^2 dx = \left[\frac{1}{3}x^3\right]_{-1}^{+1} = \frac{2}{3}$$

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- $nq = 1$: $x_{iq}^{(1)} = 0$, $w_{i_q} = 2$. $I_{gq} = 0$
- $nq = 2$: $x_q^{(1)} = -1/\sqrt{3}$, $x_q^{(2)} = 1/\sqrt{3}$, $w_q^{(1)} = w_q^{(2)} = 1$. $I_{gq} = \frac{2}{3}$

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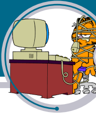
- It also works for all $n_q > 2$ !

# Numerical integration
## Gaussian quadrature, example





```
program integration
implicit none
integer, parameter:: nq=2
real(8),dimension(nq),parameter:: xq=(/-1.d0/sqrt(3.d0),+1.d0/sqrt(3.d0)/)
real(8),dimension(nq),parameter:: wq=(/1.d0,1.d0/)
real(8) I
integer iq

I=0.d0
do iq=1,nq
   I=I+wq(iq)*fct(xq(iq))
end do

write(*,*) 'I=',I

contains

function fct(x)
implicit none
real(8) x,fct

!fct=3.14
!fct=x+1
fct=x**2

end function

end program
```

# Numerical integration
## Gaussian quadrature, example



(to copy-paste)

```
program integration
implicit none
integer, parameter::  nq=2
real(8),dimension(nq),parameter::  xq=(/-1.d0/sqrt(3.d0),+1.d0/sqrt(3.d0)/)
real(8),dimension(nq),parameter::  wq=(/1.d0,1.d0/)
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I=0.d0
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I=I+wq(iq)*fct(xq(iq))
end do
write(*,*) 'I=',I
contains
function fct(x)
implicit none
real(8) x,fct
fct=x**2
end function
end program
```



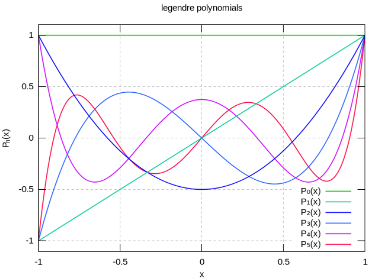
Exercise 3:

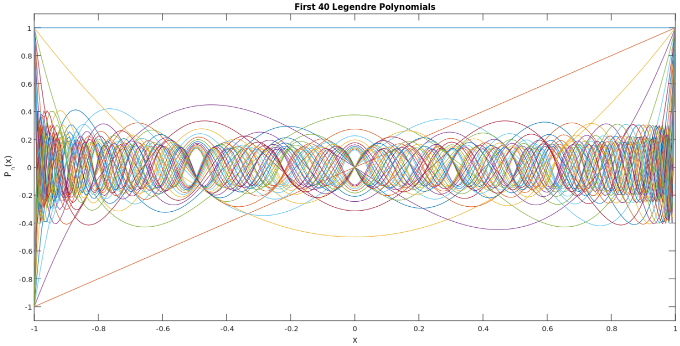
- Modify the previous program to use 5 quadrature points instead of two.
- Integrate the functions

$$f_1(x) = \sin(x\pi + \pi/2) \qquad f_2(x) = \sqrt{x+1} \qquad f_3(x) = x^4 - x^3$$

  with the 2-point and the 5-point quadrature rules.
- Compare the results with the analytical values.

- The fundamental theorem of Gaussian quadrature states that the optimal abscissas of the $n_q-$point Gaussian quadrature formulas are precisely the roots of the orthogonal polynomial for the same interval and weighting function.
- Gaussian quadrature is optimal because it fits all polynomials up to degree $2n_q - 1$ exactly.






An important property of the Legendre polynomials is that they are orthogonal with respect to the $L^2$ inner product on the interval $[-1, 1]$

$$\int_{-1}^{+1} P_m(x) P_n(x) dx = \frac{2}{2n+1} \delta_{mn}$$

# Numerical integration
## Gauss quadrature in 2D



Let us now turn to a two-dimensional integral of the form

$$I = \int_a^b \int_c^d f(x,y) dx dy$$

The equivalent Gaussian quadrature writes:

$$I_{gq} \simeq \sum_{i_q=1}^{n_q} \sum_{j_q}^{n_q} f(x_{i_q}, y_{j_q}) w_{i_q} w_{j_q}$$

Exercise 4:

- Compute analytically the following integral:

$$f(x,y) = x^2 + 4y$$

  over the domain $\Omega = [11,14] \times [7,10]$
- Write a code which integrates this function by means of a 2x2, 3x3 or 4x4 Gauss-Legendre quadrature algorithm.

# Numerical integration



Applying this to Finite Elements

**Before**

initialisation & setup
mesh domain (fill icon array)

timestepping loop

do iel=1,nel — loop over elements

- use icon array to retrieve node # which make up iel
- compute $M^e$ and $K_d^e$
- build $A^e$ and $b^e$
- assemble in A and b

apply b.c.
solve

**Now**

initialisation & setup
mesh domain (fill icon array)

timestepping loop

do iel=1,nel — loop over elements

use icon array to retrieve
node # which make up iel

do iq=1,nq — loop over quad. pts

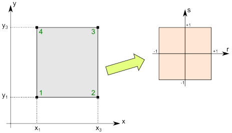
$A^e = A^e + \ldots$
$b^e = b^e + \ldots$

assemble in A and b

apply b.c.
solve

# Numerical integration
## Exercise 2

Verify the analytically derived expressions for $\boldsymbol{K}_a^e$, $\boldsymbol{K}_d^e$, and $\boldsymbol{M}^e$.




$$
\begin{aligned}
\boldsymbol{M}^e &= \int_{\Omega_e} \rho c_p \boldsymbol{N}^T \boldsymbol{N} d\Omega \\
&= \int_{x_1}^{x_3} \int_{y_1}^{y_3} \rho(x,y) c_p(x,y) \boldsymbol{N}^T(x,y) \boldsymbol{N}(x,y) dxdy \\
&= \frac{h_x h_y}{4} \int_{-1}^{+1} \int_{-1}^{+1} \rho(r,s) c_p(r,s) \boldsymbol{N}^T(r,s) \boldsymbol{N}(r,s) drds \\
&= \frac{h_x h_y}{4} \sum_{i_q} \sum_{j_q} \rho(r_{i_q}, s_{j_q}) c_p(r_{i_q}, s_{j_q}) \boldsymbol{N}^T(r_{i_q}, s_{j_q}) \boldsymbol{N}(r_{i_q}, s_{j_q}) w_{i_q} w_{j_q}
\end{aligned}
$$

# Numerical integration



$$\boldsymbol{K}_a^e = \frac{\rho c_p}{3} \begin{pmatrix} -\frac{1}{2}uh_y - \frac{1}{2}vh_x & \frac{1}{2}uh_y - \frac{1}{4}vh_x & \frac{1}{4}uh_y + \frac{1}{4}vh_x & -\frac{1}{4}uh_y + \frac{1}{2}vh_x \\ -\frac{1}{2}uh_y - \frac{1}{4}vh_x & \frac{1}{2}uh_y - \frac{1}{2}vh_x & \frac{1}{4}uh_y + \frac{1}{2}vh_x & -\frac{1}{4}uh_y + \frac{1}{4}vh_x \\ -\frac{1}{4}uh_y - \frac{1}{4}vh_x & \frac{1}{4}uh_y - \frac{1}{2}vh_x & \frac{1}{2}uh_y + \frac{1}{2}vh_x & -\frac{1}{2}uh_y + \frac{1}{4}vh_x \\ -\frac{1}{4}uh_y - \frac{1}{2}vh_x & \frac{1}{4}uh_y - \frac{1}{4}vh_x & \frac{1}{2}uh_y + \frac{1}{4}vh_x & -\frac{1}{2}uh_y + \frac{1}{2}vh_x \end{pmatrix}$$

$$
\boldsymbol{K}_d^e = k\frac{h_x h_y}{6}
\begin{pmatrix}
\frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{2}{h_x^2}+\frac{1}{h_y^2} & -\frac{1}{h_x^2}-\frac{1}{h_y^2} & \frac{1}{h_x^2}-\frac{2}{h_y^2} \\
. & \frac{2}{h_x^2}+\frac{2}{h_y^2} & \frac{1}{h_x^2}-\frac{2}{h_y^2} & -\frac{1}{h_x^2}-\frac{1}{h_y^2} \\
. & . & \frac{2}{h_x^2}+\frac{2}{h_y^2} & -\frac{2}{h_x^2}+\frac{1}{h_y^2} \\
. & . & . & \frac{2}{h_x^2}+\frac{2}{h_y^2}
\end{pmatrix}
$$

# Numerical integration



$$\boldsymbol{M}_d^e = \rho c_p \frac{h_x h_y}{9} \left( \begin{array}{cccc} 1 & 1/2 & 1/4 & 1/2 \\ . & 1 & 1/2 & 1/4 \\ . & . & 1 & 1/2 \\ . & . & . & 1 \end{array} \right)$$