CEGM1000
Modelling, Uncertainty and Data for Engineers

Week 1.5
Numerical modelling (Fundamentals)

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with A LOT of support from Isabel Slingerlad, Gabriel Follet and the rest of MUDEs' wonderful team

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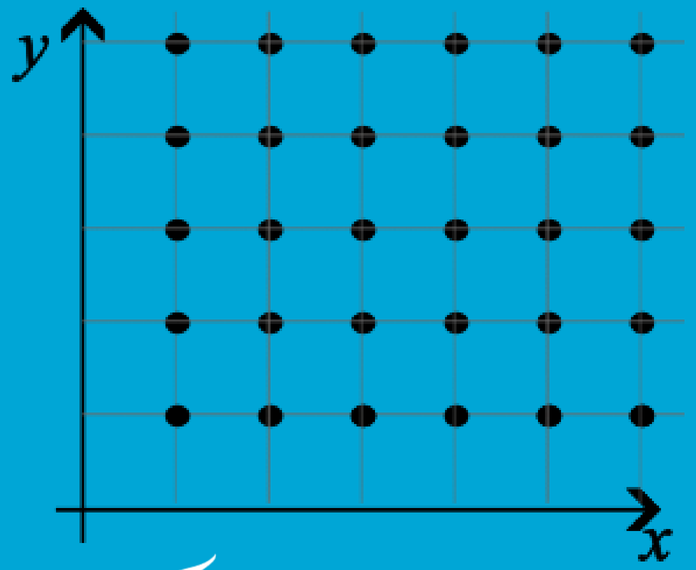
1D

$$f(x) = f(x_0) + f'(x_0)\frac{(x - x_0)}{1!} + f''(x_0)\frac{(x - x_0)^2}{2!} + \cdots$$

2D



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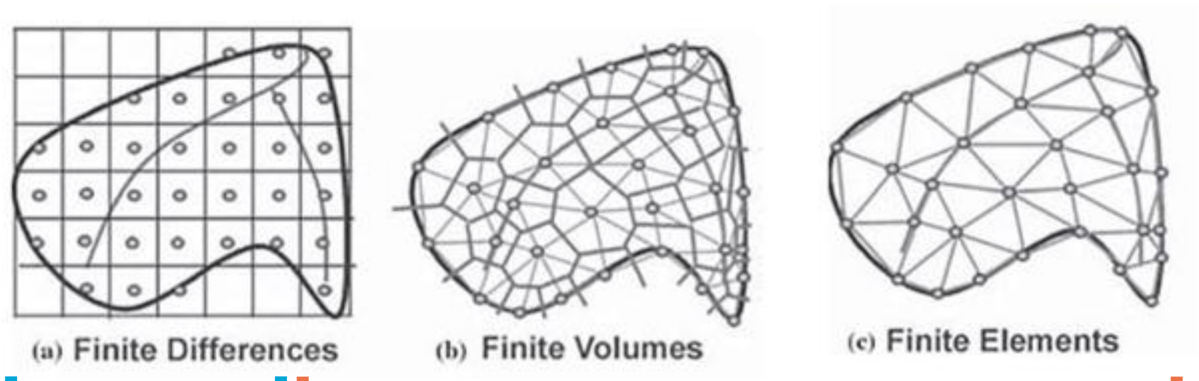
Learning objectives

At the end of this lecture, you should be able to

- Discuss the relevance of numerical modelling keeping in mind its pitfalls
- Use Taylor series to find approximations of derivatives and its accuracy
- Apply numerical integration methods to functions using pen and paper.

Methods



MUDE Q1

MUDE Q2

Q3, Q4 and beyond (depending on your path)

Other methods:

- Based on characteristics
- Boundary elements
- Physics-informed neural networks

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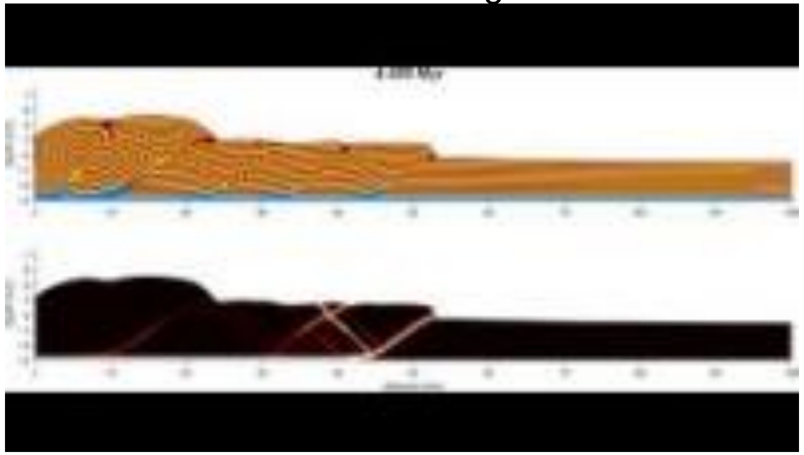
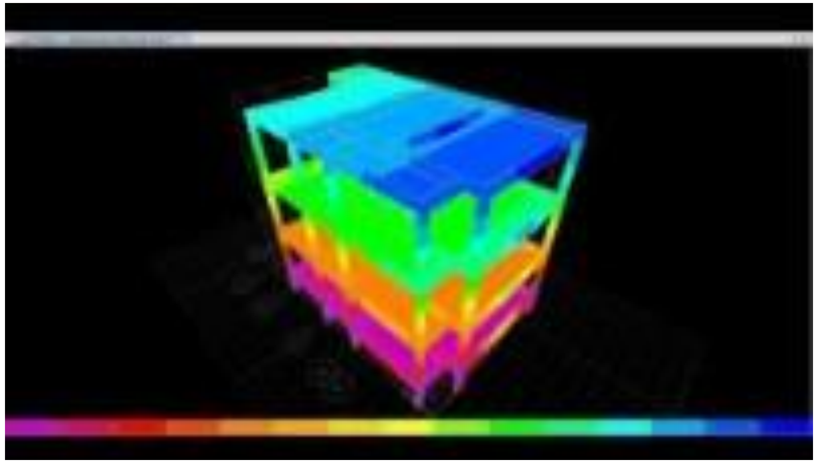
Some applications

Mountain building



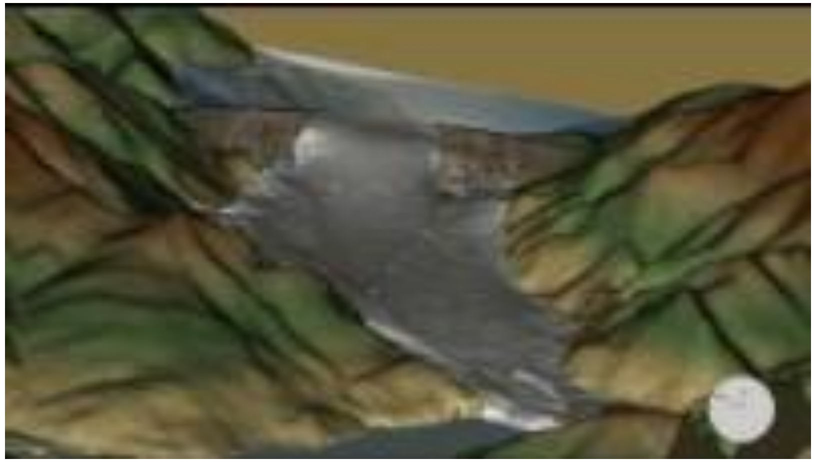
Garrett Apuzen-Ito. (2016, Nov 16). *Numerical model of mountain building* [Video]. Youtube. https://www.youtube.com/watch?v=HUn8lzdDmfk

Building Deformation



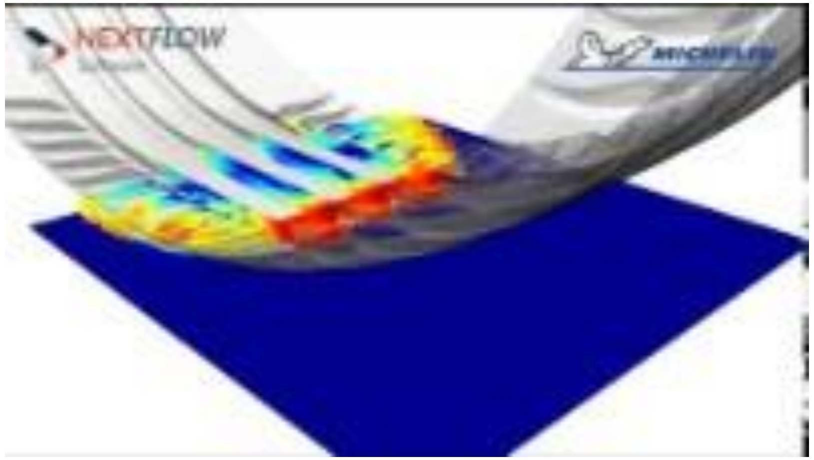
ONKAR CHAUHAN. (2018, Jan 7). *3D Animation of deformation of Building after analysis in ETABS* [Video]. Youtube. https://www.youtube.com/watch?v=RJZRtdINSms

Dam Break Simulation



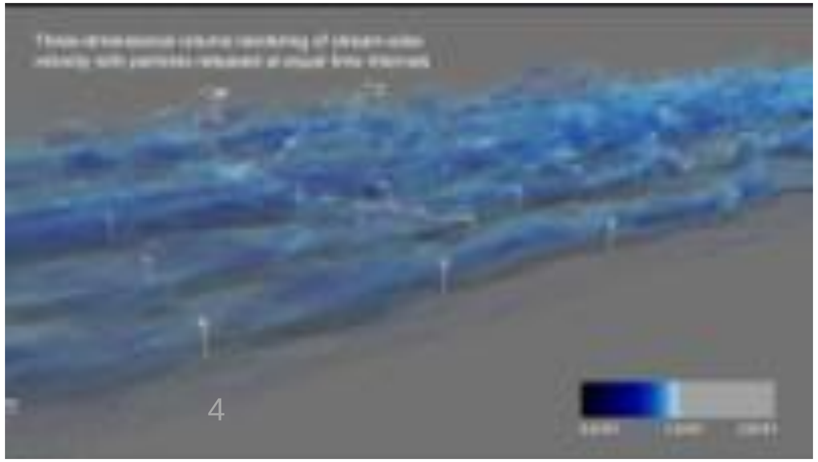
XC ENGINEERING. (2016, Mar 17). *Damn break simulation with FLOW-3D* [Video]. Youtube. https://www.youtube.com/watch?v=3q8EY4zBf3w

Tire - hydroplanning



Nextflow Software. (2019, Mar 14). *Tyre Hydroplanning simulation* [Video]. Youtubehttps://www.youtube.com/watch?v=0sVCOn_hoGU

Large eddy simulation of a Wind Farm



Physics of Fluids Group University of Twente. (2016, October 27). *Large eddy simulation of a Wind Farm- Explanatory clip* [Video]. Youtube. https://www.youtube.com/watch?v=qEtcCjln-0Q

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*Which simulation do you **feel** is more reliable?*

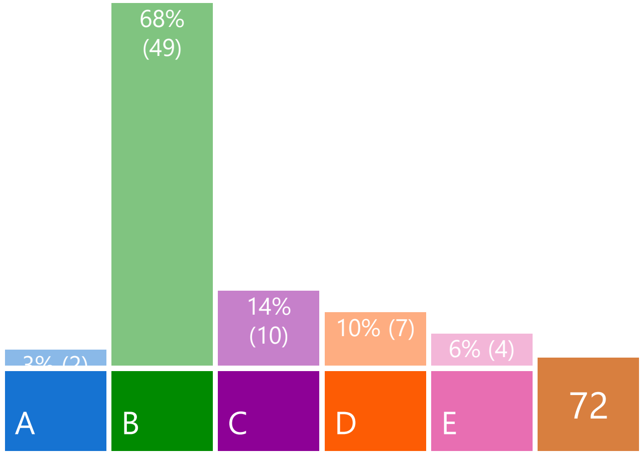
A. Mountain building

B. Structure deformation

C. Dam break

D. Hydroplanning

E. Wind field



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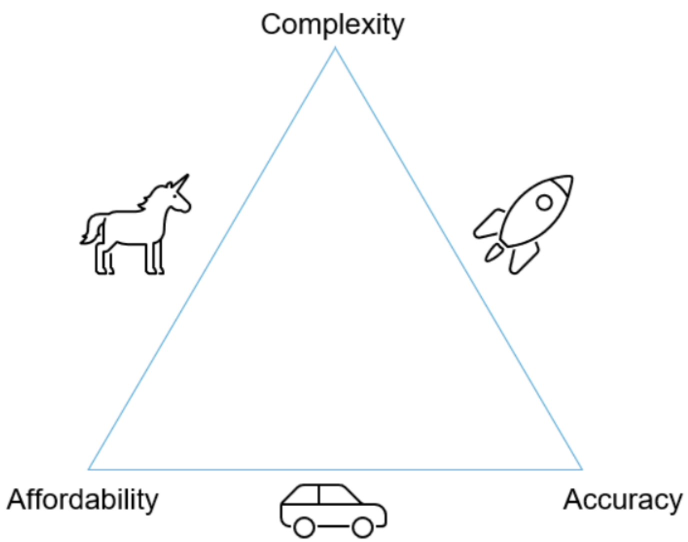
A short discussion about numerical models

All models are wrong but some are useful. "George Box"

Some Pros

1. Model future scenarios
2. Model inexistent situations
3. Some experiments cannot be scaled



Some Cons

1. They give credibility to incorrect results
2. Good modellers are scarce
3. Can consume a lot of energy

When all you have is a hammer, everything looks like a nail. "Unknown"

Differential equations –ODEs, PDEs

Ice growth
First order ODE ➔

$$\rho_{ice}\frac{dh_{ice}}{dt} = -k_{ice}\frac{T_{water} - T_{air}}{h_{ice}}$$

Beam deformation
Second order ODE ➔

$$\frac{d^2v}{dz^2} = \frac{-1}{EI}\left(-\frac{qz^2}{2} + qLz - \frac{qL^2}{2}\right)$$

Diffusion equation 1D
Second order PDE ➔

$$\frac{du}{dt} = k\frac{d^2u}{dx^2}$$

Navier Stokes 3D
System on non-linear PDEs ➔

$$\rho\left[\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}u + \frac{\partial u}{\partial y}v + \frac{\partial u}{\partial z}w\right] = -\frac{\partial p}{\partial x} + \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) + \rho g_x$$

$$\rho\left[\frac{\partial v}{\partial t} + \frac{\partial v}{\partial x}u + \frac{\partial v}{\partial y}v + \frac{\partial v}{\partial z}w\right] = -\frac{\partial p}{\partial y} + \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2}\right) + \rho g_y$$

$$\rho\left[\frac{\partial w}{\partial t} + \frac{\partial w}{\partial x}u + \frac{\partial w}{\partial y}v + \frac{\partial w}{\partial z}w\right] = -\frac{\partial p}{\partial z} + \mu\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) + \rho g_z$$

Differential equations –ODEs, PDEs

Ice growth
First order ODE ➔

$$\rho_{ice}\frac{dh_{ice}}{dt} = -k_{ice}\frac{T_{water}-T_{air}}{h_{ice}}$$

Beam c
Second

Diffusio
Second

Navier
System
linear P

$$\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\Bigg)+\rho g_x$$

$$\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\Bigg)+\rho g_y$$

$$\rho\left[\frac{\partial}{\partial t}\ \frac{\partial}{\partial x}\ \frac{\partial}{\partial y}\ \frac{\partial}{\partial z}\right]\ \frac{\partial}{\partial z}+\mu\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right)+\rho g_z$$

Approximate numerically the derivatives!

$$\frac{dh_{ice}}{dt}\approx ?$$

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Contents

Numerical Derivatives

Definition ➔ $$\left.\frac{df}{dx}\right|_{x_0} = f'(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

Numerically ➔ $$f'(x_0) \approx \frac{f(x) - f(x_0)}{\Delta x}, \text{where } \Delta x = x - x_0$$

More than one derivative (approximation)?

$$\text{forward} \left.\frac{df}{dx}\right|_{x_i} \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

$$\text{backward} \left.\frac{df}{dx}\right|_{x_i} \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

$$\text{central} \left.\frac{df}{dx}\right|_{x_i} \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$

Taylor Series Expansions

- The exact value of any function $f(x)$ can be calculated using infinite number of terms.

$$f(x) = f(x_0) + f'(x_0)\frac{(x - x_0)}{1!} + f''(x_0)\frac{(x - x_0)^2}{2!} + f'''(x_0)\frac{(x - x_0)^3}{3!} + \cdots + f^{(n)}(x_0)\frac{(x - x_0)^n}{n!}$$

Taylor Series Expansions

- Compute the Taylor Series Expansion of $f(x) = \sin(x)$ around $x_0 = 0$ until including third order of accuracy

$$f(x) = f(x_0) + f'(x_0)\frac{(x - x_0)}{1!} + f''(x_0)\frac{(x - x_0)^2}{2!} + f'''(x_0)\frac{(x - x_0)^3}{3!}$$

$\mathrm{f}(0) = \sin(0) \longrightarrow \mathrm{f}(0) = 0$

$\mathrm{f}'(0) = \cos(0) \longrightarrow \mathrm{f}'(0) = 1$

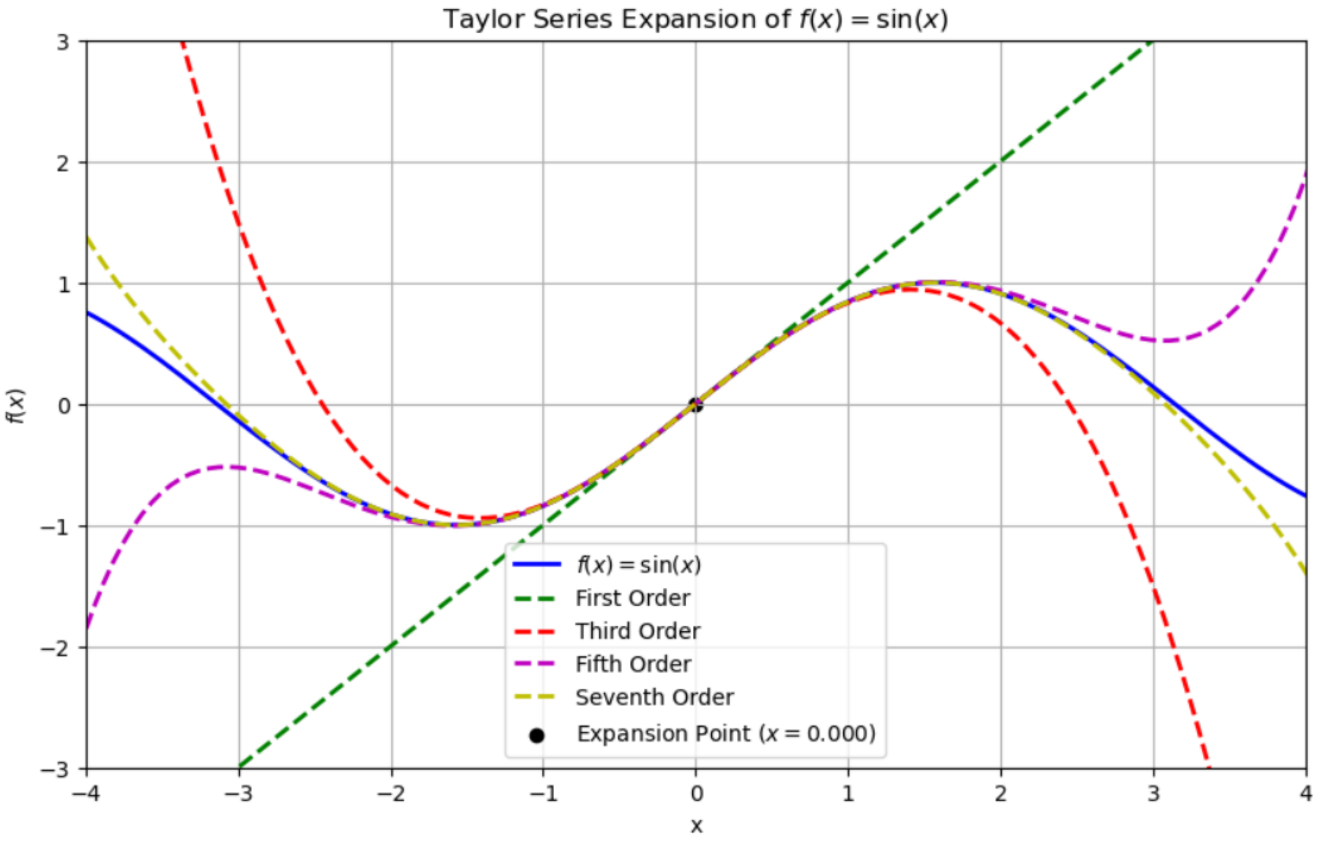
$\mathrm{f}''(0) = -\sin(0) \longrightarrow \mathrm{f}''(0) = 0$

$\mathrm{f}'''(0) = -\cos(0) \longrightarrow \mathrm{f}'''(0) = -1$

Taylor Series Expansions

- Compute the Taylor Series Expansion of $f(x) = \sin(x)$ around $x_0 = 0$ until including third order of accuracy

$$\sin(x) = x - \frac{x^3}{6}$$



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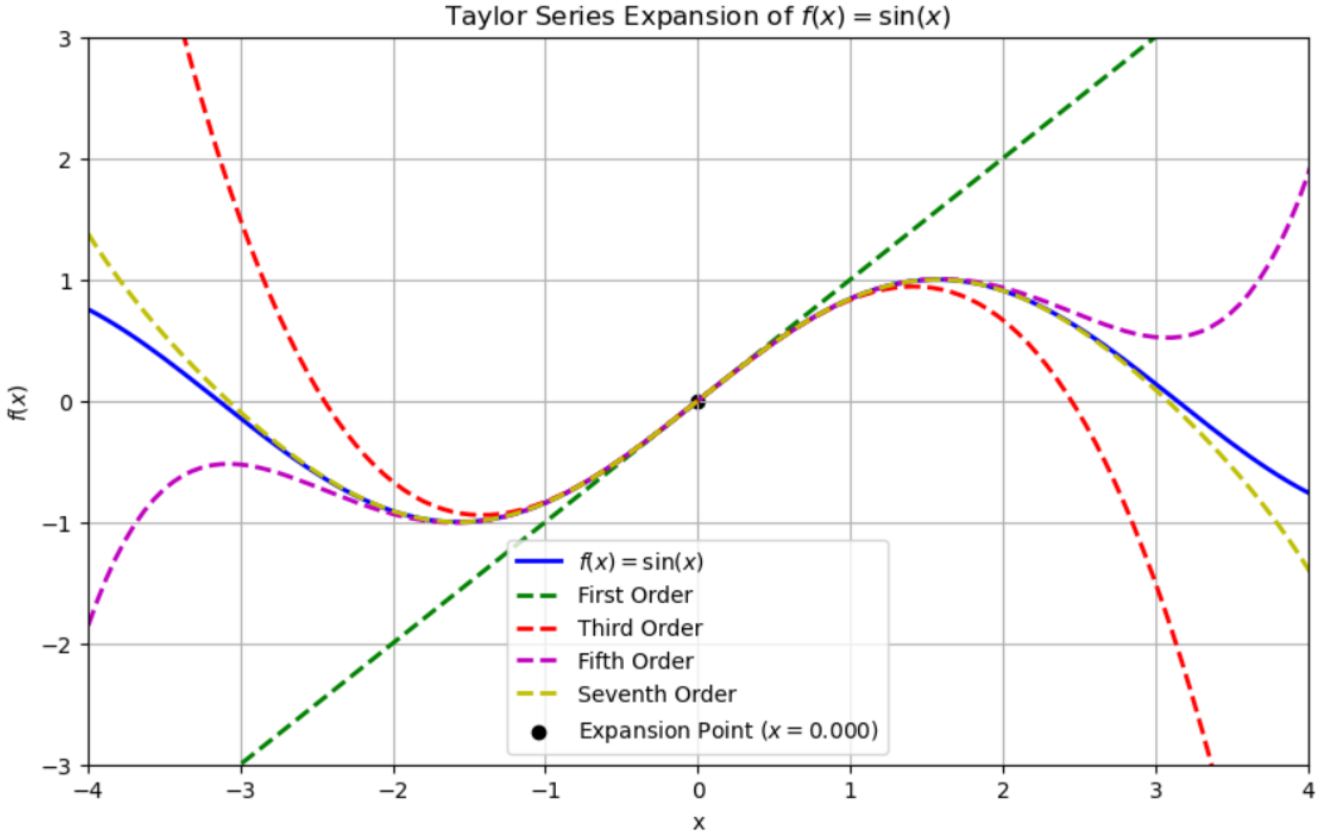
At x = 10 which approximation gives the best result (least worse)?

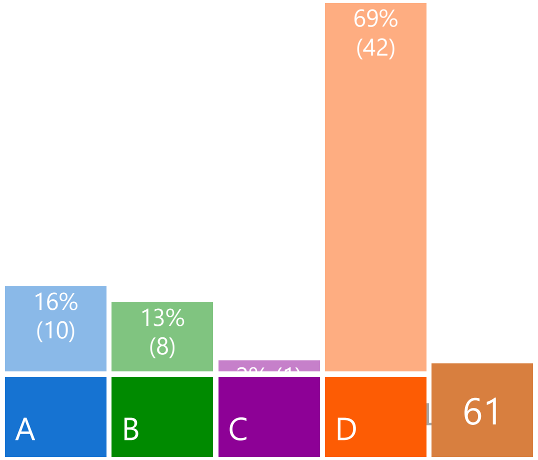
A. 1 term

B. 3 terms

C. 5 terms

D. 7 terms





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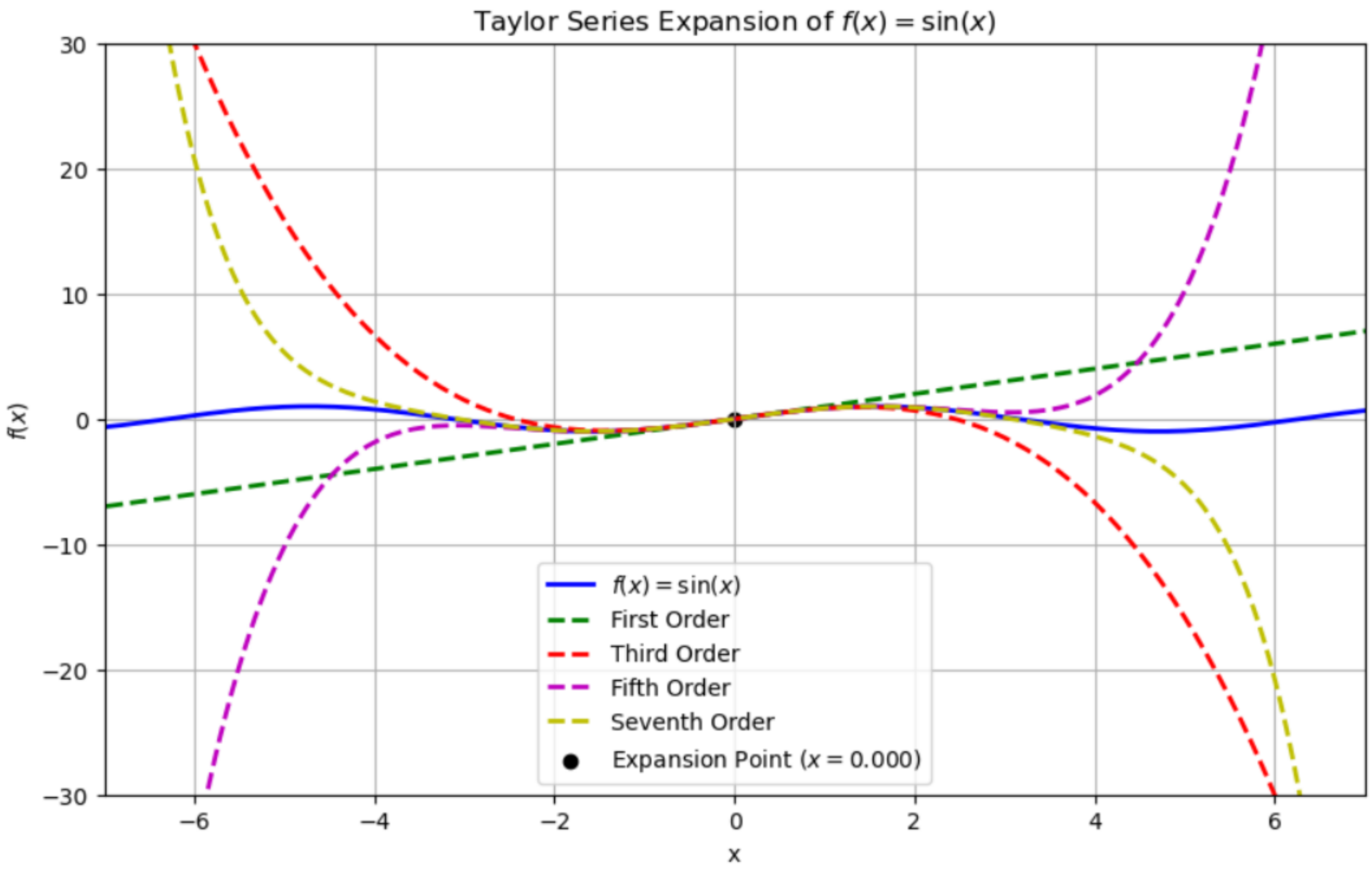
- The more terms used; the solution will be more accurate near x_0
- The farther from x_0; the error increases



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Taylor Series Expansions to get the derivatives

- Basic derivatives
- Higher order FD
- Second derivative FD

Taylor Series Expansions to get the derivatives

- Different numerical **approximations** of the derivative can be found using TSE
- Using TSE we also find the error order. FD/BD are first-order accurate, CD second-order accurate
- You can find **more accurate approximations** by using more points
- The approximation of the second derivative requires at least one more point of information

Taylor expansion – 2 variables

- Taylor series for a function of one variable y=f(x):

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \cdots + \frac{f^n(x_0)}{n!}(x - x_0)^n$$

- Second degree Taylor Polynomial of a function of two variables, f(x,y)

$$f(x,y) \approx f(x_0, y_0) + f'_x(x_0, y_0)(x - x_0) + f'_y(x_0, y_0)(y - y_0) + \frac{f''_x(x_0,y_0)}{2}(x - x_0)^2 + \frac{f''_y(x_0,y_0)}{2}(y - y_0)^2$$
$$+ f''_{xy}(x_0, y_0)(x - x_0)(y - y_0)$$

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*What kind of relationship do you **expect** to have with models?*

A. Decision taker

B. User

C. Superuser

D. Developer/Creator

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*What kind of relationship do you **expect** to have with models?*

A. Decision taker

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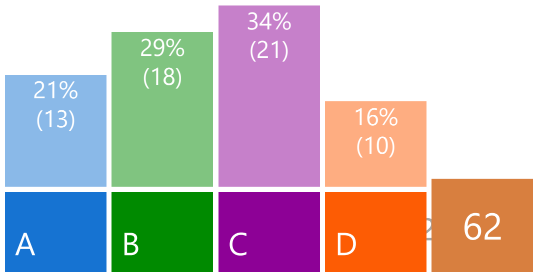

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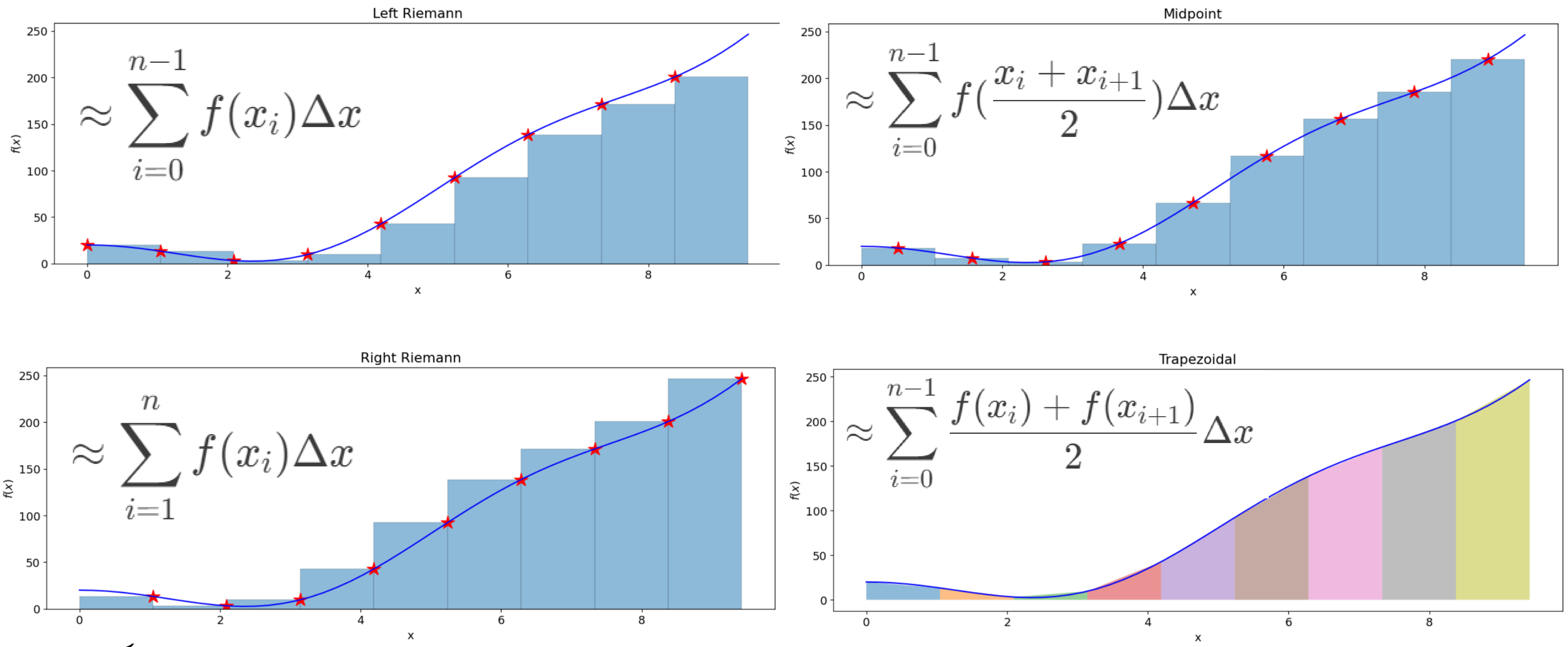
Numerical Integration Rules

Numerical integration : a technique used to approximate the value of a defined integral, when it is not possible to obtain the exact value.

Numerical integration rules :

- Left Riemann
- Right Riemann
- Midpoint rule
- Trapezoidal rule
- Simpsons rule

Numerical integration methods: $I \approx$



Numerical Integration Rules

$$\text{Left Riemann Error} = |\bar{f}'(b-a)\Delta x/2| \text{ therefore } \mathcal{O}(\Delta x)$$

$$\text{Right Riemann Error} = |\bar{f}'(b-a)\Delta x/2| \text{ therefore } \mathcal{O}(\Delta x)$$

$$\text{Midpoint Error} = |\bar{f}''(b-a)\Delta x^2/2| \text{ therefore } \mathcal{O}(\Delta x^2)$$

$$\text{Trapezoidal Error} = |\bar{f}''(b-a)\Delta x^2/2| \text{ therefore } \mathcal{O}(\Delta x^2)$$

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