Numerical Integration of Partial Differential Equations (PDEs)

- Introduction to PDEs.
- Stationary Problems, Elliptic PDEs.
- Time dependent Problems.
- Complex Problems in Solar System Research.
Introduction to PDEs.

• Definition of Partial Differential Equations.
• Second Order PDEs.
  - Elliptic
  - Parabolic
  - Hyperbolic
• Linear, nonlinear and quasi-linear PDEs.
• What is a well posed problem?
• Boundary value Problems (stationary).
• Initial value problems (time dependent).
Differential Equations

• A differential equation is an equation for an unknown function of one or several variables that relates the values of the function itself and of its derivatives of various orders.

• Ordinary Differential Equation: Function has 1 independent variable.

• Partial Differential Equation: At least 2 independent variables.
Physical systems are often described by coupled Partial Differential Equations (PDEs)

- Maxwell equations
- Navier-Stokes and Euler equations in fluid dynamics.
- MHD-equations in plasma physics
- Einstein-equations for general relativity
  - ...
  - ...

...
PDEs definitions

- General (implicit) form for one function \( u(x,y) \):
  \[
  F \left( x, y, u(x,y), \frac{\partial u(x,y)}{\partial x}, \frac{\partial u(x,y)}{\partial y}, \ldots, \frac{\partial^2 u(x,y)}{\partial x \partial y}, \ldots \right) = 0,
  \]

- Highest derivative defines order of PDE

- Explicit PDE => We can resolve the equation to the highest derivative of \( u \).

- Linear PDE => PDE is linear in \( u(x,y) \) and for all derivatives of \( u(x,y) \)

- Semi-linear PDEs are nonlinear PDEs, which are linear in the highest order derivative.
Linear PDEs of 2. Order

\[ a(x,y) \frac{\partial^2 u(x,y)}{\partial x^2} + b(x,y) \frac{\partial^2 u(x,y)}{\partial x \partial y} + c(x,y) \frac{\partial^2 u(x,y)}{\partial y^2} \]

\[ + d(x,y) \frac{\partial u(x,y)}{\partial x} + e(x,y) \frac{\partial u(x,y)}{\partial y} + f(u,x,y) = 0 \]

- \( a(x,y)c(x,y) - b(x,y)2 / 4 > 0 \) Elliptic
- \( a(x,y)c(x,y) - b(x,y)2 / 4 = 0 \) Parabolic
- \( a(x,y)c(x,y) - b(x,y)2 / 4 < 0 \) Hyperbolic

Quasi-linear: coefficients depend on \( u \) and/or first derivative of \( u \), but NOT on second derivatives.
PDEs and Quadratic Equations

- Quadratic equations in the form

\[ Ax^2 + Bxy + Cy^2 + Dx + Ey + F = 0 \]

describe cone sections.

- \( a(x,y)c(x,y) - b(x,y)^2 / 4 > 0 \) Ellipse
- \( a(x,y)c(x,y) - b(x,y)^2 / 4 = 0 \) Parabola
- \( a(x,y)c(x,y) - b(x,y)^2 / 4 < 0 \) Hyperbola
With coordinate transformations these equations can be written in the standard forms:

Ellipse: \[ \frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \]

Parabola: \[ y^2 = 4ax \]

Hyperbola: \[ \frac{x^2}{a^2} - \frac{y^2}{b^2} = 1 \]

Coordinate transformations can be also applied to get rid of the mixed derivatives in PDEs. (For space dependent coefficients this is only possible locally, not globally)
Parabola- cutting plane parallel to side of cone.

Circle and Ellipse

Hyperbolas
Linear PDEs of 2. Order

\[ a(x,y) \frac{\partial^2 u(x,y)}{\partial x^2} + b(x,y) \frac{\partial^2 u(x,y)}{\partial x \partial y} + c(x,y) \frac{\partial^2 u(x,y)}{\partial y^2} + d(x,y) \frac{\partial u(x,y)}{\partial x} + e(x,y) \frac{\partial u(x,y)}{\partial y} + f(u, x, y) = 0 \]

- Please note: We still speak of linear PDEs, even if the coefficients \(a(x,y)\) ... \(e(x,y)\) might be nonlinear in \(x\) and \(y\).
- Linearity is required only in the unknown function \(u\) and all derivatives of \(u\).
- Further simplification are:
  - constant coefficients \(a\)-\(e\),
  - vanishing mixed derivatives \((b=0)\)
  - no lower order derivatives \((d=e=0)\)
  - a vanishing function \(f=0\).
Second Order PDEs with more than 2 independent variables

\[ Lu = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{i,j} \frac{\partial^2 u}{\partial x_i \partial x_j} \text{ plus lower order terms} = 0. \]

Classification by eigenvalues of the coefficient matrix:

- **Elliptic:** All eigenvalues have the same sign. [Laplace-Eq.]
- **Parabolic:** One eigenvalue is zero. [Diffusion-Eq.]
- **Hyperbolic:** One eigenvalue has opposite sign. [Wave-Eq.]
- **Ultrahyperbolic:** More than one positive and negative eigenvalue.

Mixed types are possible for non-constant coefficients, appear frequently in science and are often difficult to solve.
Elliptic Equations

• Occurs mainly for stationary problems.
• Solved as boundary value problem.
• Solution is smooth if boundary conditions allow.

Example: Poisson and Laplace-Equation (f=0)

\[ \nabla^2 \Phi = f \]

\[ \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2} \Phi(x) = f(x) \]
Parabolic Equations

- The vanishing eigenvalue often related to time derivative.
- Describes non-stationary processes.
- Solved as Initial- and Boundary-value problem.
- Discontinuities / sharp gradients smooth out during temporal evolution.

Example: Diffusion-Equation, Heat-conduction

\[
\frac{\partial}{\partial t} u(x, t) = a \cdot \frac{\partial^2}{\partial x^2} u(x, t) \quad \frac{\partial}{\partial t} u(\vec{r}, t) = a \cdot \Delta u(\vec{r}, t)
\]
Hyperbolic Equations

- The opposite sign eigenvalue is often related to the time derivative.
- Initial- and Boundary value problem.
- Discontinuities / sharp gradients in initial state remain during temporal evolution.
- A typical example is the Wave equation.

\[ c^2 \frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 u}{\partial t^2} \left( \Delta - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) u = 0 \]

- With nonlinear terms involved sharp gradients can form during the evolution =&gt; Shocks
Well posed problems
(as defined by Hadamard 1902)

A problem is well posed if:

• A solution exists.
• The solution is unique.
• The solution depends continuously on the data (boundary and/or initial conditions).

Problems which do not fulfill these criteria are ill-posed.

Well posed problems have a good chance to be solved numerically with a stable algorithm.
Ill-posed problems

• Ill-posed problems play an important role in some areas, for example for inverse problems like tomography.
• Problem needs to be reformulated for numerical treatment.
• => Add additional constraints, for example smoothness of the solution.
• Input data need to be regularized / preprocessed.
Ill-conditioned problems

• Even well posed problems can be **ill-conditioned**.
• $=>$ Small changes (errors, noise) in data lead to large errors in the solution.
• Can occur if continuous problems are solved approximately on a numerical grid.
  PDE $=>$ algebraic equation in form $Ax = b$
• **Condition number** of matrix $A$:

$$\kappa(A) = \frac{\lambda_{\text{max}}(A)}{\lambda_{\text{min}}(A)}$$

$\lambda_{\text{max}}(A), \lambda_{\text{min}}(A)$ are maximal and minimal eigenvalues of $A$.
• Well conditioned problems have a **low condition number**.
How to solve PDEs?

- PDEs are solved together with appropriate **Boundary Conditions** and/or **Initial Conditions**.

- **Boundary value problem**
  - Dirichlet B.C.: Specify $u(x,y,...)$ on boundaries (say at $x=0$, $x=L_x$, $y=0$, $y=L_y$ in a rectangular box)
  - von Neumann B.C.: Specify normal gradient of $u(x,y,...)$ on boundaries.

In principle boundary can be arbitrary shaped.
(but difficult to implement in computer codes)
Boundary value problem
• **Initial value problem**

  • Boundary values are usually specified on all boundaries of the computational domain.
  • Initial conditions are specified in the entire computational (spatial) domain, but only for the initial time \( t=0 \).
  • Initial conditions as a Cauchy problem:

    - Specify initial distribution \( u(x,y,...,t=0) \) [for parabolic problems like the Heat equation]
    - Specify \( u \) and \( du/dt \) for \( t=0 \) [for hyperbolic problems like wave equation.]
Initial value problem

boundary conditions

initial values
Cauchy Boundary conditions

- Cauchy B.C. impose both Dirichlet and Von Neumann B.C. on part of the boundary (for PDEs of 2. order).
- More general: For PDEs of order \( n \) the Cauchy problem specifies \( u \) and all derivatives of \( u \), up to the order \( n-1 \) on parts of the boundary.
- In physics the Cauchy problem is often related to temporal evolution problems (initial conditions specified for \( t=0 \)).

Augustin Louis Cauchy
1789-1857
Introduction to PDEs
Summary

• What is a well posed problem? Solution exists, is unique, continuous on boundary conditions.
• **Elliptic** (Poisson), **Parabolic** (Diffusion) and **Hyperbolic** (Wave) PDEs.
• PDEs are solved with **boundary conditions** and **initial conditions**.
• What are **Dirichlet** and **von Neumann** boundary conditions?
Numerical Integration of Partial Differential Equations (PDEs)

- Semi-analytic methods to solve PDEs.
Semi-analytic methods to solve PDEs.

- From systems of coupled first order PDEs (which are difficult to solve) to uncoupled PDEs of second order.
- Example: From Maxwell equations to wave equation.
- (Semi) analytic methods to solve the wave equation by separation of variables.
- Exercise: Solve Diffusion equation by separation of variables.
How to obtain uncoupled 2. order PDEs from physical laws?

• Example: From Maxwell equations to wave equations.
• Maxwell equations are a coupled system of first order vector PDEs.
• Can we reformulate this equations to a more simple form?
• Here we use the electromagnetic potentials, vector potential and scalar potential.
Maxwell equations

\[ \nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} \]

\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \]

\[ \nabla \cdot \mathbf{B} = 0 \]

\[ \nabla \cdot \mathbf{E} = \frac{1}{\epsilon_0} \rho \]

James C. Maxwell
1831-1879
Maxwell Equations:

\[ \nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \varepsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} \]
\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \]
\[ \nabla \cdot \mathbf{B} = 0 \]
\[ \nabla \cdot \mathbf{E} = \frac{1}{\varepsilon_0} \rho \]

We use the electromagnetic potentials

\[ \mathbf{B} = \nabla \times \mathbf{A} \]
\[ \mathbf{E} = -\nabla \Phi - \frac{\partial \mathbf{A}}{\partial t} \]

together with the Lorenz Gauge condition (after Ludvig Lorenz 1829-1891). Lorenz Gauge is often wrongly referred to as Lorentz Gauge (after Hendrik Lorentz, who made many discoveries in electro dynamics, but has nothing to do with the Lorenz Gauge.)

\[ \nabla \cdot \mathbf{A} + \frac{1}{c^2} \frac{\partial \Phi}{\partial t} = 0 \]
With these definitions we get:

\[ \nabla \times \nabla \times \mathbf{A} = \mu_0 \mathbf{j} + \epsilon_0 \mu_0 \frac{\partial}{\partial t} \left( -\nabla \Phi - \frac{\partial \mathbf{A}}{\partial t} \right) \]

\[ \nabla \times \left( -\nabla \Phi - \frac{\partial \mathbf{A}}{\partial t} \right) = -\frac{\partial \nabla \times \mathbf{A}}{\partial t} \quad \checkmark \]

\[ \nabla \cdot \nabla \times \mathbf{A} = 0 \quad \checkmark \]

\[ \nabla \cdot \left( -\nabla \Phi - \frac{\partial \mathbf{A}}{\partial t} \right) = \frac{1}{\epsilon_0} \rho \]

We use the vector identity \( \nabla \times \nabla \times \mathbf{A} = \nabla (\nabla \cdot \mathbf{A}) - \Delta \mathbf{A} \)

and the definition \( \epsilon_0 \mu_0 = \frac{1}{c^2} \)

\[ \nabla (\nabla \cdot \mathbf{A}) - \Delta \mathbf{A} = \mu_0 \mathbf{j} + \frac{1}{c^2} \frac{\partial}{\partial t} \left( -\nabla \Phi - \frac{\partial \mathbf{A}}{\partial t} \right) \]

\[ -\Delta \Phi - \frac{\partial (\nabla \cdot \mathbf{A})}{\partial t} = \frac{1}{\epsilon_0} \rho \]
After reordering the terms in the first equation:
\[
\nabla \left( \nabla \cdot \mathbf{A} + \frac{1}{c^2} \frac{\partial \Phi}{\partial t} \right) - \Delta \mathbf{A} + \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} = \mu_0 j \\
-\Delta \Phi - \frac{\partial (\nabla \cdot \mathbf{A})}{\partial t} = \frac{1}{\epsilon_0 \rho}
\]

Finally we use the Lorentz Gauge and derive Wave equations:

\[
-\Delta \mathbf{A} + \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} = \mu_0 j \\
-\Delta \Phi + \frac{1}{c^2} \frac{\partial^2 \Phi}{\partial t^2} = \frac{1}{\epsilon_0 \rho}
\]
What do we win with wave equations?

- Inhomogenous coupled system of Maxwell reduces to wave equations.
- We get 2. order scalar PDEs for components of electric and magnetic potentials.
- Equation are not coupled and have same form.
- Well known methods exist to solve these wave equations.
Wave equation

• Electric charges and currents on right side of wave-equation can be computed from other sources:
• Moments of electron and ion-distribution in space-plasma.
• The particle-distributions can be derived from numerical simulations, e.g. by solving the Vlasov equation for each species.
• Here we study the wave equation in vacuum for simplicity.
Wave equation in vacuum

\[ -\Delta A + \frac{1}{c^2} \frac{\partial^2 A}{\partial t^2} = 0 \]

\[ -\Delta \Phi + \frac{1}{c^2} \frac{\partial^2 \Phi}{\partial t^2} = 0 \]
(Semi-) analytic methods

- Example: Homogenous wave equation

\[-\Delta \Phi + \frac{1}{c^2} \frac{\partial^2 \Phi}{\partial t^2} = 0\]

- Can be solved by any analytic function \(f(x-ct)\) and \(g(x+ct)\).

- As the homogenous wave equation is a linear equation any linear combination of \(f\) and \(g\) is also a solution of the PDE.

- This property can be used to specify boundary and initial conditions. The appropriate coefficients have to be found often numerically.
Semi-analytic method: Variable separation

\[ c^2 \frac{\partial^2 \Phi}{\partial x^2} = \frac{\partial^2 \Phi}{\partial t^2} \]

We define: \( \frac{\partial^2 \Phi}{\partial x^2} \equiv \Phi'' \), \( \frac{\partial^2 \Phi}{\partial t^2} \equiv \ddot{\Phi} \)

Solve PDE by separation of variables:

\[ \Phi(x, t) = \Phi_1(t) \cdot \Phi_2(x) \]

\[ \Rightarrow c^2 \Phi_1 \cdot \Phi_2'' = \ddot{\Phi}_1 \Phi_2 \quad \text{Divide by} \quad c^2 \Phi_1 \Phi_2 \]

\[ \Rightarrow \frac{\Phi_2''}{\Phi_2} = \frac{1}{c^2} \frac{\ddot{\Phi}_1}{\Phi_1} = -k^2 \quad \text{Arbitrary constant} \ k. \]

Left side is only function of \( x \) and right only of \( t \).
\[ \Phi''_2 = -k^2 \Phi_2, \quad \Phi'_1 = -k^2 c^2 \Phi_1 \]

The ODEs have the solutions:

\[ \Phi_2 = \exp(\pm i k x), \quad \Phi_1 = \exp(\pm i k c t) \]

Or if you do not like complex functions:

\[ \Phi_2 = \sin(kx), \cos(kx), \quad \Phi_1 = \sin(kc t), \cos(kc t) \]

Any combination (4 possibilities) is a solution of our PDE! We normalize \( k \) with the box length \( L_x \) by \( \hat{k} = \frac{2\pi}{L_x} k \)

Let’s talk about Boundary Conditions. For example:

\[ \Phi(0, t) = \Phi(L_x, t) = 0 \Rightarrow \cos(kx) \text{ terms eliminated.} \]
Semi-analytic method: Variable separation

Now let's apply initial conditions for $\Phi$ and $\dot{\Phi}$

$$\Phi(x, 0) = \rho(x) \text{ (arbitrary)} \text{ and } \dot{\Phi}(x, 0) = 0$$

$$\dot{\Phi}(x, 0) = 0 \Rightarrow \sin(ktc) \text{ terms eliminated.}$$

A particular solution of the PDE is:

$$\Phi_k(x, t) = \sin\left(\frac{k\pi}{L_x} x\right) \cdot \cos\left(\frac{kc\pi}{L_x} t\right)$$

Our PDE is linear $\Rightarrow$
Superposition of particular solutions is also a solution:

$$\Phi(x, t) = \sum_{k=0}^{\infty} a_k \cdot \sin\left(\frac{k\pi}{L_x} x\right) \cdot \cos\left(\frac{kc\pi}{L_x} t\right)$$
Semi-analytic method: Variable separation

How to apply the initial condition $\Phi(x, 0) = \rho(x)$?

Fourier series: $\Phi(x, 0) = \sum_{k=0}^{\infty} a_k \cdot \sin \left( \frac{k\pi}{L_x} x \right)$

with $a_k = \frac{2}{L_x} \int_0^{L_x} \sin \left( \frac{k\pi}{L_x} x \right) \cdot \rho(x) \, dx$

Provides us the required initial conditions and fixes the coefficients $a_k$. Usually we have to evaluate the integral for $a_k$ numerically. (That’s why we call the method semi-analytic). For practical computations we do not use an infinity number of modes $k$, but maximal the number of grid points $n_x$ in the $x$-direction.

$\Phi(x, t) = \sum_{k=0}^{n_x} a_k \cdot \sin \left( \frac{k\pi}{L_x} x \right) \cdot \cos \left( \frac{k\pi c}{L_x} t \right)$
Semi-analytic method: Variable separation

Show: demo_wave_sep.pro

This is an IDL-program to animate the wave-equation
Exercise:
1D diffusion equation

lecture_diffusion_draft.pro

This is a draft IDL-program to solve the diffusion equation by separation of variables.

Task: Find separable solutions for Dirichlet and von Neumann boundary conditions and implement them.
Semi-analytic methods

Summary

• Some (mostly) linear PDEs with constant coefficients can be solved analytically.

• One possibility is the method ‘Separation of variables’, which leads to ordinary differential equations.

• For linear PDEs.: Superposition of different solutions is also a solution of the PDE.
Numerical Integration of Partial Differential Equations (PDEs)

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- Semi-analytic methods to solve PDEs.
- Introduction to Finite Differences.
  - Stationary Problems, Elliptic PDEs.
  - Time dependent Problems.
  - Complex Problems in Solar System Research.

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Introduction to Finite Differences.

• Remember the definition of the differential quotient.
• How to compute the differential quotient with a finite number of grid points?
• First order and higher order approximations.
• Central and one-sided finite differences.
• Accuracy of methods for smooth and not smooth functions.
• Higher order derivatives.
Numerical methods

• Most PDEs cannot be solved analytically.
• Variable separation works only for some simple cases and in particular usually not for inhomogenous and/or nonlinear PDEs.
• Numerical methods require that the PDE become discretized on a grid.
• **Finite difference methods** are popular/most commonly used in science. They replace differential equation by difference equations)
• Engineers (and a growing number of scientists too) often use **Finite Elements.**
Finite differences

Remember the definition of differential quotient:

\[
\frac{df(x)}{dx} = f'(x) = \lim_{h \to 0} \frac{f(x + h) - f(x)}{h}
\]

- How to compute differential quotient numerically?
- Just apply the formular above for a finite \( h \).
- For simplicity we use an equidistant grid in \( x=[0,h,2h,3h,\ldots,(n-1)\ h] \) and evaluate \( f(x) \) on the corresponding grid points \( x_i \).
- Grid resolution \( h \) must be sufficient high. Depends strongly on function \( f(x) \)!
Accuracy of finite differences

We approximate the derivative of \( f(x) = \sin(n \cdot x) \) on a grid \( x = 0 \ldots 2 \pi \) with 50 (and 500) grid points by

\[
\frac{df}{dx} = \frac{f(x+h) - f(x)}{h}
\]

and compare with the exact solution \( \frac{df}{dx} = n \cos(n \cdot x) \)

Average error done by discretisation:
- 50 grid points: 0.040
- 500 grid points: 0.004
Accuracy of finite differences

We approximate the derivative of \( f(x) = \sin(n \cdot x) \) on a grid \( x=0 \ldots 2 \pi \) with 50 (and 500) grid points by 
\[
\frac{df}{dx} = \frac{f(x+h) - f(x)}{h}
\]
and compare with the exact solution \( \frac{df}{dx} = n \cos(n \cdot x) \)

Average error done by discretisation:
50 grid points: 2.49
500 grid points: 0.256
Higher accuracy methods

Can we use more points for higher accuracy?
Higher accuracy: Central differences

- \( \frac{df}{dx} = \frac{(f(x+h) - f(x))}{h} \) computes the derivative at \( x+h/2 \) and not exactly at \( x \).

- The alternative formula \( \frac{df}{dx} = \frac{(f(x) - f(x-h))}{h} \) has the same shortcomings.

- We introduce **central differences**: 
  \( \frac{df}{dx} = \frac{(f(x+h) - f(x-h))}{2h} \) which provides the derivative at \( x \).

- Central differences are of 2. order accuracy instead of 1. order for the simpler methods above.
How to find higher order formulars?

For sufficient smooth functions we describe the function $f(x)$ locally by polynomial of $n$th order. To do so $n+1$ grid points are required. $n$ defines the order of the scheme.

Make a Taylor expansion (Definition $x_{i+1} = x_i + \Delta x$):

\[
\begin{align*}
    f_{i+1} &= f_i + \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) + \frac{\Delta x^3}{6} f'''(x_i) + O(\Delta x^4) \\
    f_{i-1} &= f_i - \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) - \frac{\Delta x^3}{6} f'''(x_i) + O(\Delta x^4) \\
    f_{i+2} &= f_i + 2\Delta x f'(x_i) + 2\Delta x^2 f''(x_i) + \frac{4\Delta x^3}{3} f'''(x_i) + O(\Delta x^4)
\end{align*}
\]
How to find higher order formulas?

And by linear combination we get the central difference:

\[ f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + O(\Delta x^2) \]

At boundary points central differences might not be possible (because the point i-1 does not exist at the boundary i=0), but we can still find schemes of the same order by one-sited (here right-sited) derivative:

\[ f'(x_i) = \frac{4f_{i+1} - f_{i+2} - 3f_i}{2\Delta x} + O(\Delta x^2) \]

Alternatives to one sited derivatives are periodic boundary conditions or to introduce ghost-cells.
Higher derivatives

How to derive higher derivatives?
From the Taylor expansion

\[ f_{i+1} = f_i + \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) + \frac{\Delta x^3}{6} f'''(x_i) + O(\Delta x^4) \]

\[ f_{i-1} = f_i - \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) - \frac{\Delta x^3}{6} f'''(x_i) + O(\Delta x^4) \]

we derive by a linear combination:

\[ f''(x_i) = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} + O(\Delta x^2) \]

Basic formula used to discretise 2.order Partial Differential Equations
Higher order methods

By using more points (higher order polynomials) to approximate $f(x)$ locally we can get higher orders, e.g. by an appropriate combination of

\[
\begin{align*}
    f_{i+1} &= f_i + \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) + \frac{\Delta x^3}{6} f'''(x_i) + \frac{\Delta x^4}{24} f^{(4)}(x_i) + O(\Delta x^5) \\
    f_{i+2} &= f_i + 2\Delta x f'(x_i) + 2\Delta x^2 f''(x_i) + \frac{4\Delta x^3}{3} f'''(x_i) + \frac{2\Delta x^4}{3} f^{(4)}(x_i) + O(\Delta x^5) \\
    f_{i-1} &= f_i - \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) - \frac{\Delta x^3}{6} f'''(x_i) + \frac{\Delta x^4}{24} f^{(4)}(x_i) + O(\Delta x^5) \\
    f_{i-2} &= f_i - 2\Delta x f'(x_i) + 2\Delta x^2 f''(x_i) - \frac{4\Delta x^3}{3} f'''(x_i) + \frac{2\Delta x^4}{3} f^{(4)}(x_i) + O(\Delta x^5)
\end{align*}
\]

we get 4th order central differences:

\[
f'(x_i) = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12\Delta x} + O(\Delta x^4)
\]
**Accuracy of finite differences**

We approximate the derivative of \( f(x) = \sin(nx) \) on a grid \( x=0 \ldots 2\pi \) with 50 (and 500) grid points with 1th, 2th and 4th order schemes:

<table>
<thead>
<tr>
<th>( n )</th>
<th>1th order</th>
<th>2th order</th>
<th>4th order</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, 50 pixel</td>
<td>0.04</td>
<td>0.0017</td>
<td>5.4 ( 10^{-6} )</td>
</tr>
<tr>
<td>1, 500 pixel</td>
<td>0.004</td>
<td>1.7 ( 10^{-5} )</td>
<td>4.9 ( 10^{-6} )</td>
</tr>
<tr>
<td>8, 50 pixel</td>
<td>2.49</td>
<td>0.82</td>
<td>0.15</td>
</tr>
<tr>
<td>8, 500 pixel</td>
<td>0.26</td>
<td>0.0086</td>
<td>4.5 ( 10^{-5} )</td>
</tr>
<tr>
<td>20, 50 pixel</td>
<td>13.5</td>
<td>9.9</td>
<td>8.1</td>
</tr>
<tr>
<td>20, 500 pixels</td>
<td>1.60</td>
<td>0.13</td>
<td>0.0017</td>
</tr>
</tbody>
</table>
What scheme to use?

- Higher order schemes give significant better results only for problems which are smooth with respect to the used grid resolution.
- Implementation of high order schemes makes more effort and take longer computing time, in particular for solving PDEs.
- Popular and a kind of standard are second order methods.
- If we want to feed our PDE-solver with (usually unsmooth) observed data higher order schemes can cause additional problems.
Summary

- Differential quotient is approximated by finite differences on a discrete numerical grid.
- Popular are in particular central differences, which are second order accurate.
- The grid resolution should be high enough, so that the discretized functions appear smooth. => Physical gradients should be on larger scales as the grid resolution.