Numerical Integration of Partial Differential Equations (PDEs)

- Introduction to PDEs.
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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

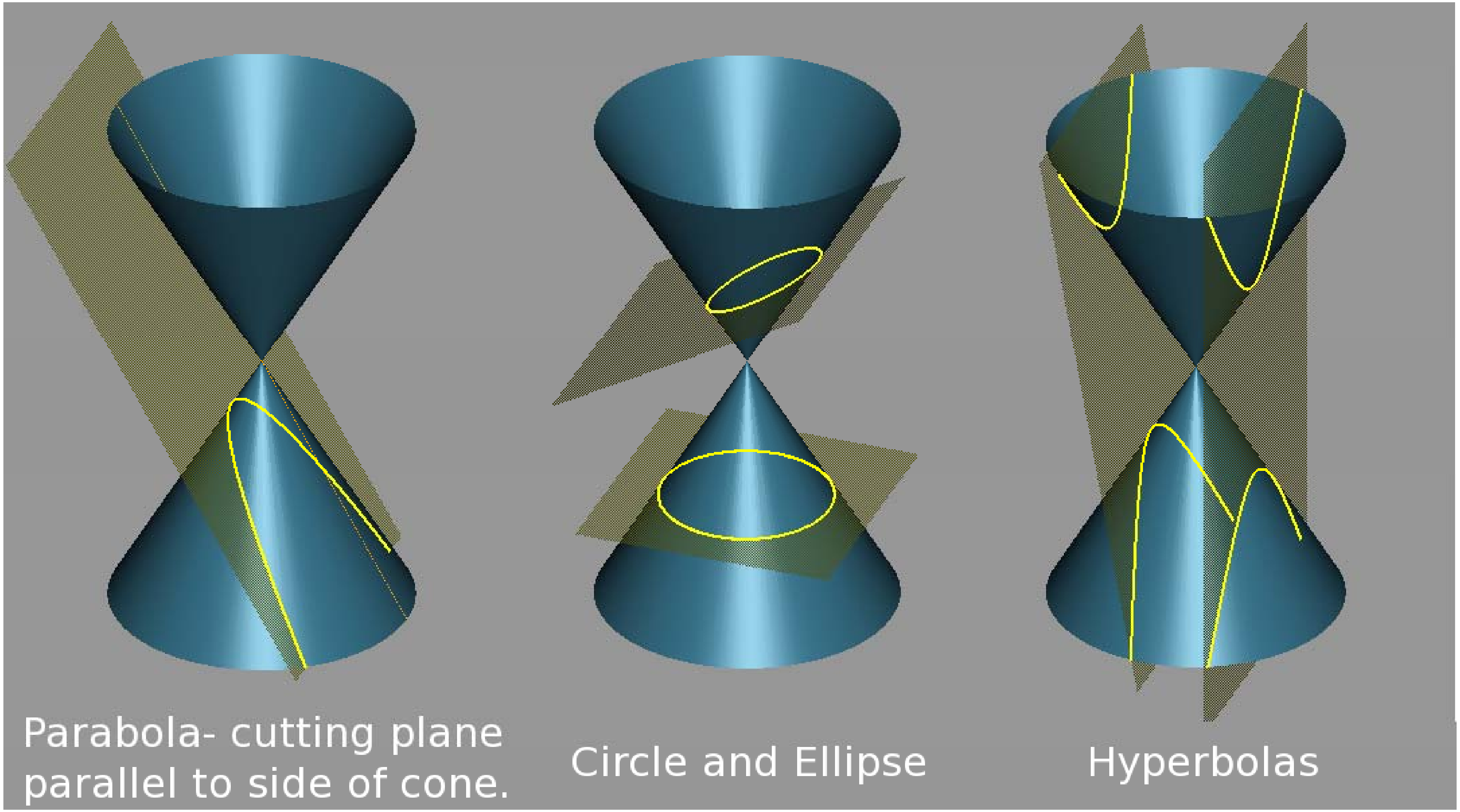
With coordinate transformations these equations can be written in the standard forms:

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 derivates (d=e=0)
  -a vanishing function f=0.

Second Order PDEs with more then 2 independent variables

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

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

$$\frac{\partial}{\partial t}u(x,t) = a \cdot \frac{\partial^2}{\partial x^2}u(x,t) \qquad \frac{\partial}{\partial t}u(\vec{r},t) = a \cdot \Delta u(\vec{r},t)$$

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.

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

- With nonlinear terms involved sharp gradients can form during the evolution => 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:

$$\kappa(A) = \left| \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} \right|$$

$\lambda_{\max}(A),\ \lambda_{\min}(A)$ are maximal and minimal eigenvalues of A.

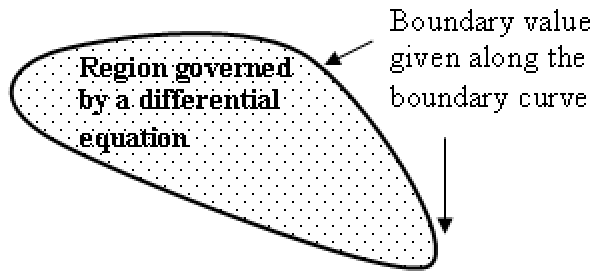
- Well conditioned problems have a **low condition number**.

How to solve PDEs?

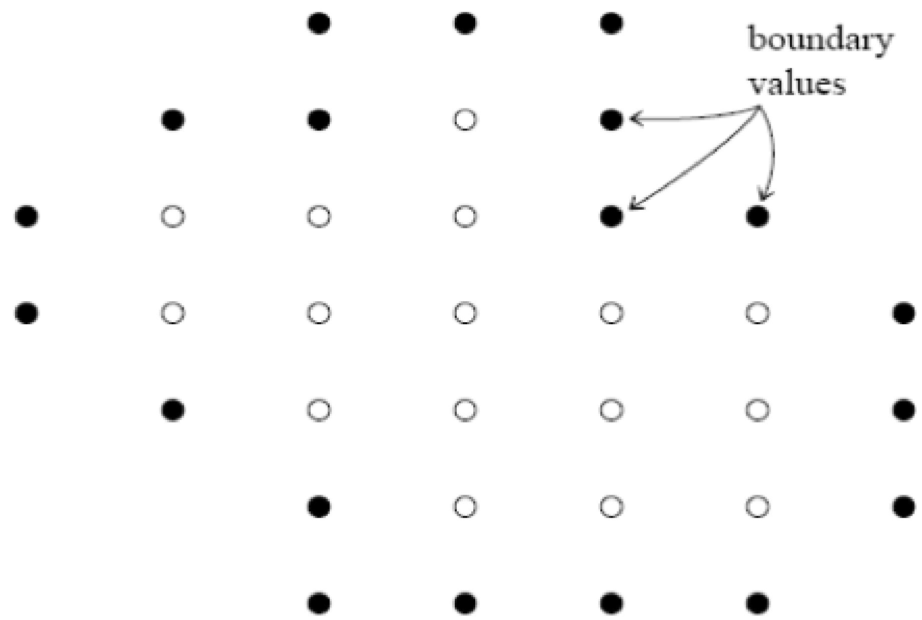
- PDEs are solved together with appropriate **Boundary Conditions** and/or **Initial Conditions**.
- **Boundary value problem**
  -**Dirichlet B.C.:** Specify u(x,y,...) on boundaries (say at x=0, x=Lx, y=0, y=Ly in a rectangular box)
  -**von Neumann B.C.:** Specify normal gradient of u(x,y,...) on boundaries.

In principle boundary can be arbitrary shaped.

(but difficult to implement in computer codes)



Boundary value problem

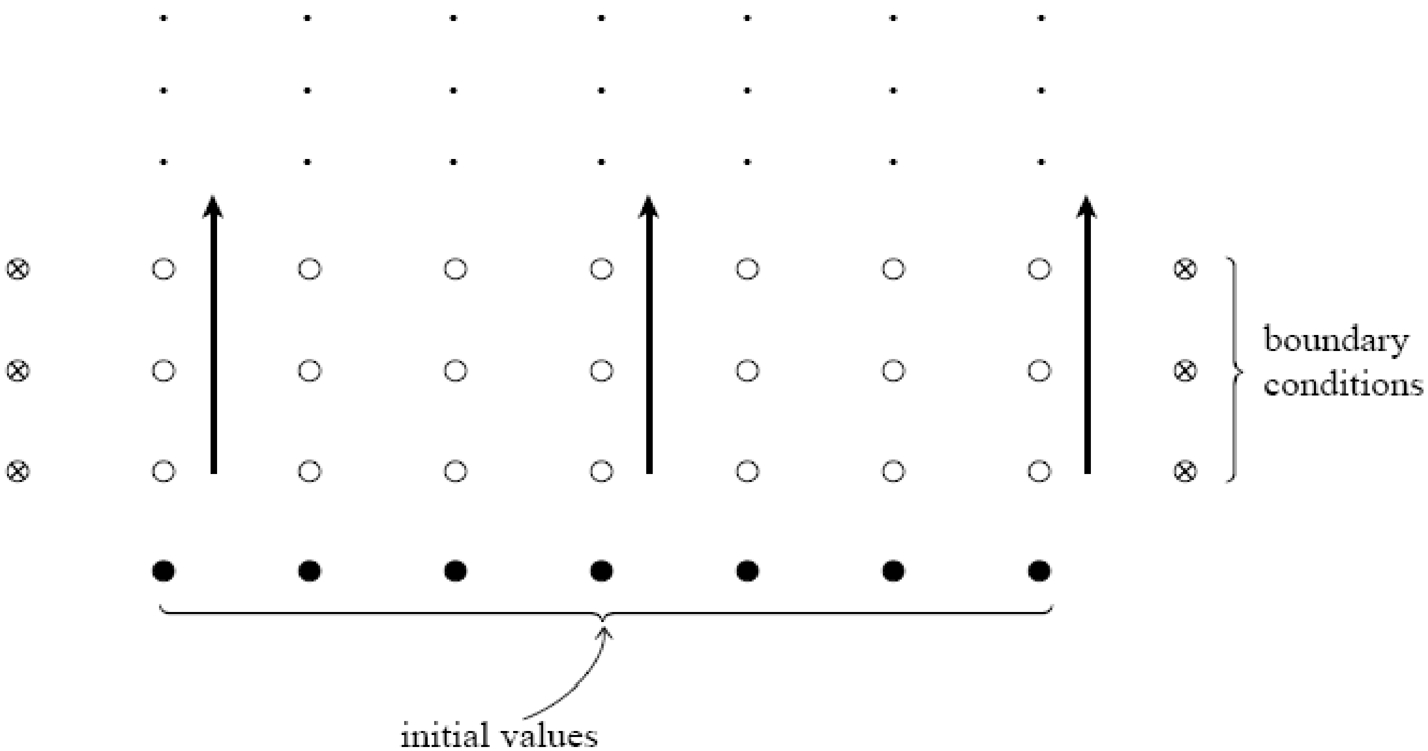


- **Initial value problem**
- Boundary values are usually specified on all boundaries of the computational domain.
- Initial conditions are specified in the entire computational (spatial) domain, but only for the initial time t=0.
- Initial conditions as a Cauchy problem:

  -Specify initial distribution u(x,y,...,t=0)
  [for parabolic problems like the Heat equation]

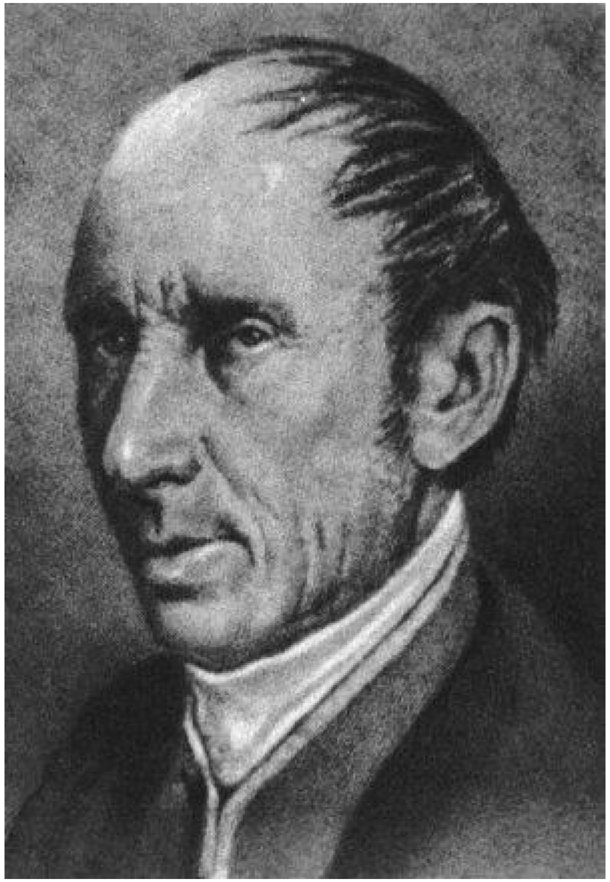
  - Specify u and du/dt for t=0
  [for hyperbolic problems like wave equation.]

Initial value problem



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)

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- Semi-analytic methods to solve PDEs.
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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, vectorpotential 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:

$$\begin{aligned}
\nabla \times \mathbf{B} &= \mu_0 \mathbf{j} + \epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} \\
\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \cdot \mathbf{E} &= \frac{1}{\epsilon_0} \rho
\end{aligned}$$

We use the electromagnetic potentials

$$\begin{aligned}
\mathbf{B} &= \nabla \times \mathbf{A} \\
\mathbf{E} &= -\nabla \mathbf{\Phi} - \frac{\partial \mathbf{A}}{\partial t}
\end{aligned}$$

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.)

$$\nabla \cdot \mathbf{A} + \frac{1}{c^2} \frac{\partial \mathbf{\Phi}}{\partial t} = 0$$

With these definitions we get:

$$
\begin{aligned}
\nabla \times \nabla \times \mathbf{A} &= \mu_0 \mathbf{j} + \epsilon_0 \mu_0 \frac{\partial}{\partial t}\left(-\nabla \mathbf{\Phi} - \frac{\partial \mathbf{A}}{\partial t}\right) \\
\nabla \times (-\nabla \mathbf{\Phi} - \frac{\partial \mathbf{A}}{\partial t}) &= -\frac{\partial \nabla \times \mathbf{A}}{\partial t} \checkmark \\
\nabla \cdot \nabla \times \mathbf{A} &= 0 \checkmark \\
\nabla \cdot (-\nabla \mathbf{\Phi} - \frac{\partial \mathbf{A}}{\partial t}) &= \frac{1}{\epsilon_0}\rho
\end{aligned}
$$

We use the vector identity $\nabla \times \nabla \times \mathbf{A} = \nabla(\nabla \cdot \mathbf{A}) - \Delta \mathbf{A}$ and the definition $\epsilon_0 \mu_0 = \frac{1}{c^2}$

$$
\begin{aligned}
\nabla(\nabla \cdot \mathbf{A}) - \Delta \mathbf{A} &= \mu_0 \mathbf{j} + \frac{1}{c^2}\frac{\partial}{\partial t}\left(-\nabla \mathbf{\Phi} - \frac{\partial \mathbf{A}}{\partial t}\right) \\
-\Delta \mathbf{\Phi} - \frac{\partial(\nabla \cdot \mathbf{A})}{\partial t} &= \frac{1}{\epsilon_0}\rho
\end{aligned}
$$

After reordering the terms in the first equation:

$$\begin{aligned}\nabla\left(\nabla\cdot\mathbf{A}+\frac{1}{c^2}\frac{\partial\mathbf{\Phi}}{\partial t}\right)-\Delta\mathbf{A}+\frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} &= \mu_0\mathbf{j}\\ -\Delta\mathbf{\Phi}-\frac{\partial(\nabla\cdot\mathbf{A})}{\partial t} &= \frac{1}{\epsilon_0}\rho\end{aligned}$$

Finally we use the Lorenz Gauge and derive Wave equations:

$$\boxed{\begin{aligned}-\Delta\mathbf{A}+\frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} &= \mu_0\mathbf{j}\\ -\Delta\mathbf{\Phi}+\frac{1}{c^2}\frac{\partial^2\Phi}{\partial t^2} &= \frac{1}{\epsilon_0}\rho\end{aligned}}$$

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

$$
\begin{aligned}
-\Delta \mathbf{A} + \frac{1}{c^2}\frac{\partial^2 \mathbf{A}}{\partial t^2} &= 0 \\
-\Delta \mathbf{\Phi} + \frac{1}{c^2}\frac{\partial^2 \Phi}{\partial t^2} &= 0
\end{aligned}
$$

(Semi-) analytic methods

- Example: Homogenous wave equation

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

- 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

$$\boxed{c^2 \frac{\partial^2 \Phi}{\partial x^2} = \frac{\partial^2 \Phi}{\partial t^2}}$$

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:

$$\Phi(x,t) = \Phi_1(t) \cdot \Phi_2(x)$$

$\Rightarrow c^2 \Phi_1 \cdot \Phi_2'' = \ddot{\Phi}_1 \Phi_2$ Devide by $c^2 \Phi_1 \Phi_2$

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

Left side is only function of x and right only of t.

$$\boxed{\Phi_2'' = -k^2\Phi_2, \quad \ddot{\Phi}_1 = -k^2\, c^2\Phi_1}$$

The ODEs have the solutions:

$$\Phi_2 = \exp(\pm i\, kx), \quad \Phi_1 = \exp(\pm i\, kc\, t)$$

Or if you do not like complex functions:

$$\boxed{\Phi_2 = \sin(kx), \cos(kx), \quad \Phi_1 = \sin(kc\, t), \cos(kc\, t)}$$

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 lets apply initial conditions for Φ and $\dot{\Phi}$

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

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

A particular solution of the PDE is:

$$\boxed{\Phi_k(x,t) = \sin(\tfrac{k\pi}{L_x}x) \cdot \cos(\tfrac{kc\pi}{L_x}t)}$$

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

$$\Phi(x,t) = \sum_{k=0}^{\infty} a_k \cdot \sin(\tfrac{k\pi}{L_x}x) \cdot \cos(\tfrac{kc\pi}{L_x}t)$$

Semi-analytic method: Variable separation

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

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

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

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.

$$\boxed{\Phi(x,t) = \sum_{k=0}^{n_x} a_k \cdot \sin(\frac{k\pi}{L_x}\, x) \cdot \cos(\frac{kc\pi}{L_x}\, t)}$$

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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- Introduction to Finite Differences.
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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

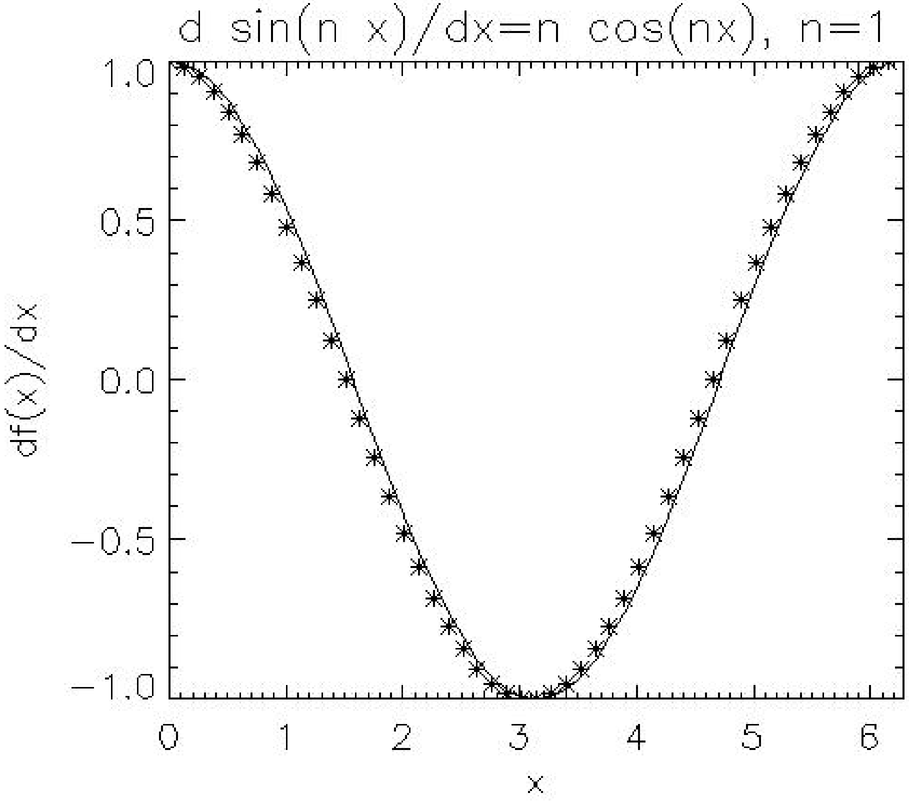
Remember the definition of differential quotient:

$$\frac{df(x)}{dx} = f'(x) = \lim_{h \longrightarrow 0} \frac{f(x+h) - f(x)}{h}$$

- 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,......(n-1) h] and evaluate f(x) on the corresponding grid points xi.
- Grid resolution h must be sufficient high. Depends strongly on function f(x)!

Accuracy of finite differences

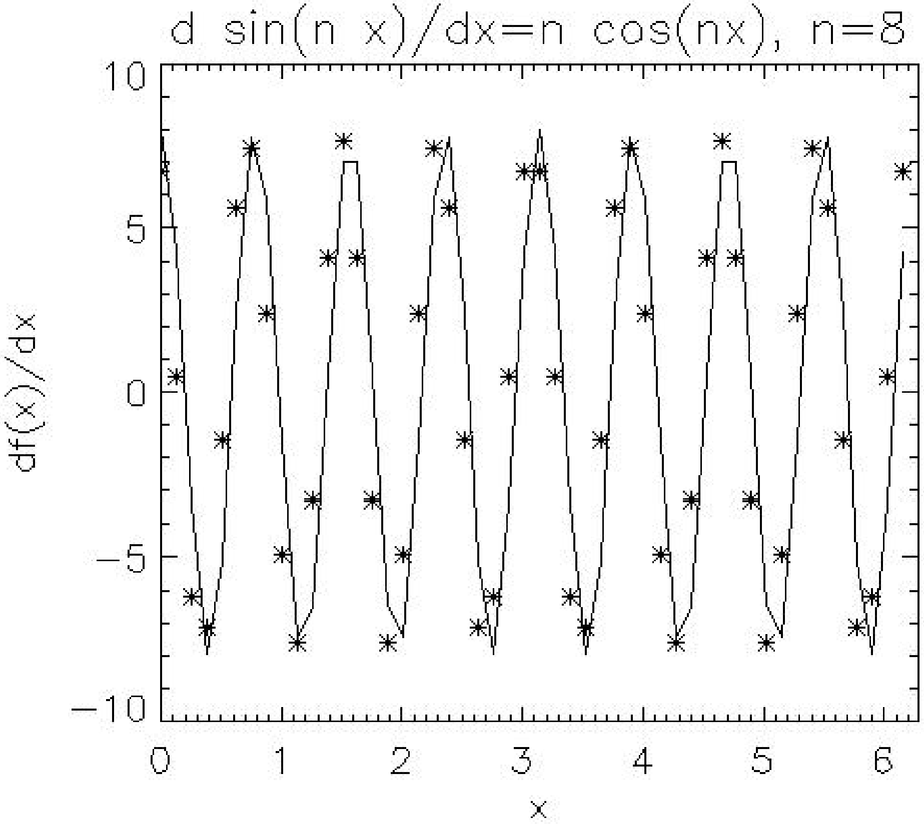
We approximate the derivative of f(x)=sin(n x) on a grid x=0 ...2 Pi with 50 (and 500) grid points by **df/dx=(f(x+h)-f(x))/h** and compare with the exact solution df/dx= n cos(n x)



Average error done by discretisation:
50 grid points: 0.040
500 grid points: 0.004

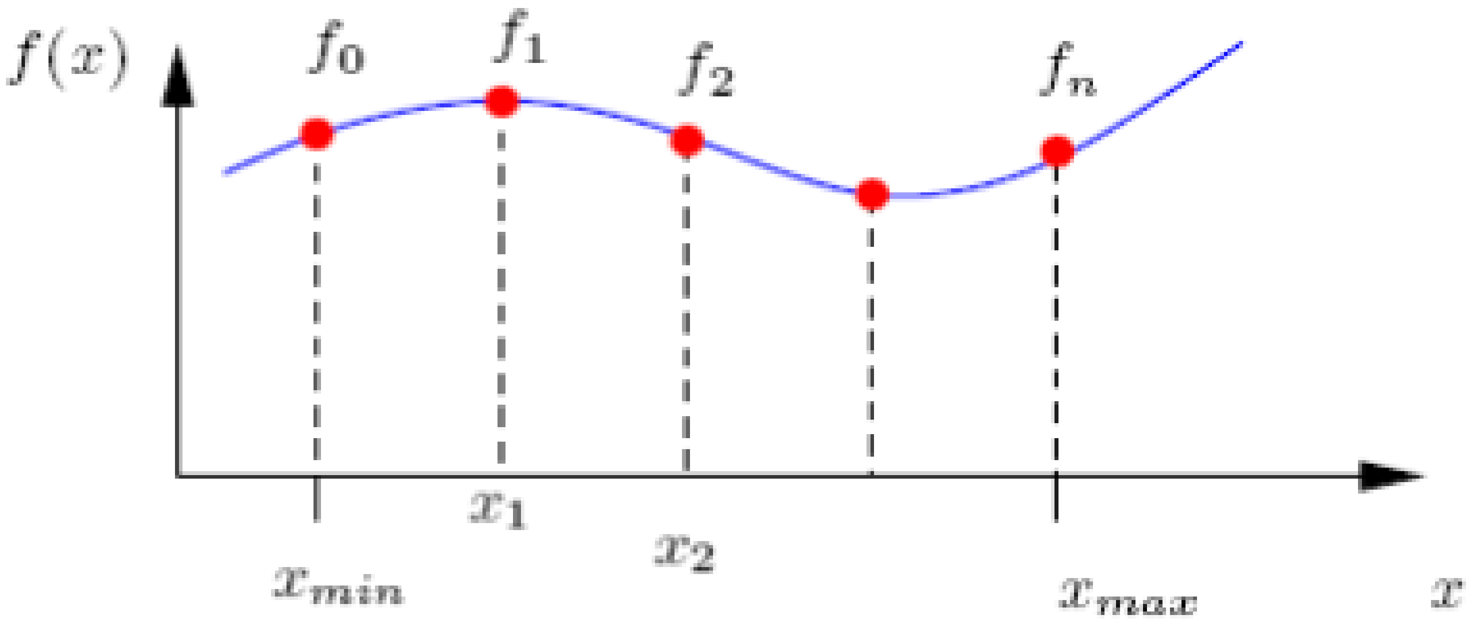
Accuracy of finite differences

We approximate the derivative of f(x)=sin(n x) on a grid x=0 ...2 Pi with 50 (and 500) grid points by **df/dx=(f(x+h)-f(x))/h** and compare with the exact solution df/dx= n cos(n 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

- df/dx=(f(x+h)-f(x))/h computes the derivative at x+h/2 and not exactly at x.
- The alternative formular df/dx=(f(x)-f(x-h))/h has the same shortcomings.
- We introduce **central differences**: **df/dx=(f(x+h)-f(x-h))/(2 h)** 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 $x_{i+1} = x_i + \Delta x$):

$$
\begin{aligned}
f_{i+1} &= f_i + \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) + \frac{\Delta x^3}{6} f'''(x_i) + O(\Delta x^4) \\
f_{i-1} &= f_i - \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) - \frac{\Delta x^3}{6} f'''(x_i) + O(\Delta x^4) \\
f_{i+2} &= f_i + 2\Delta x f'(x_i) + 2\Delta x^2 f''(x_i) + \frac{4\Delta x^3}{3} f'''(x_i) + O(\Delta x^4)
\end{aligned}
$$

How to find higher order formulars?

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

$$
\begin{aligned}
f_{i+1} &= f_i + \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) + \frac{\Delta x^3}{6} f'''(x_i) + O(\Delta x^4) \\
f_{i-1} &= f_i - \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) - \frac{\Delta x^3}{6} f'''(x_i) + O(\Delta x^4)
\end{aligned}
$$

we derive by a linear combination:

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

Basic formular used to discretise
2.order Partial Differencial 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

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

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(n x) on a grid x=0 ...2 Pi with 50 (and 500) grid points with 1th, 2th and 4th order schemes:

	1th order	**2th order**	**4th order**
n=1, 50 pixel	0.04	0.0017	$5.4\ 10^{-6}$
n=1, 500 pixel	0.004	$1.7\ 10^{-5}$	$4.9\ 10^{-6}$
n=8, 50 pixel	2.49	0.82	0.15
n=8, 500 pixel	0.26	0.0086	$4.5\ 10^{-5}$
n=20, 50 pixel	13.5	9.9	8.1
n=20, 500 pix.	1.60	0.13	0.0017

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.

Finite differences
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.