

Simulation and Analysis of 1D Wave Propagation under Various Physical Models

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DI PADOVA



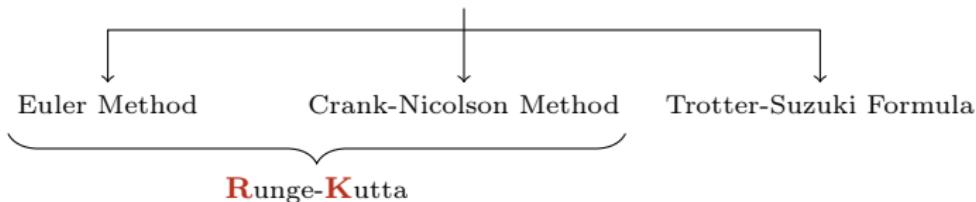
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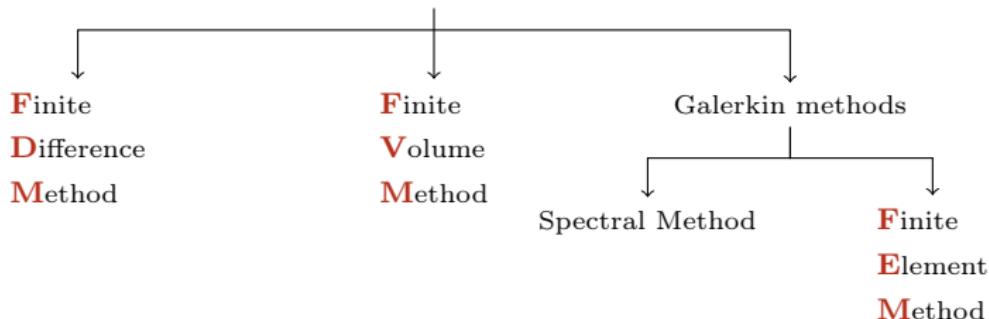
Course of **Quantum Information and Computing**
Academic Year 2024/2025

Numerical methods for differential equations

Ordinary Differential Equations

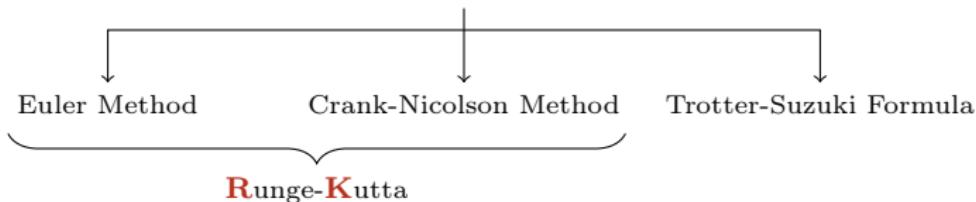


Partial Differential Equations

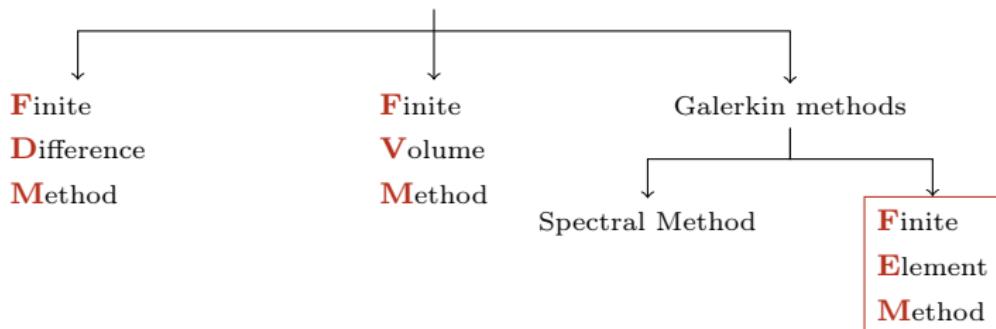


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Partial Differential Equations



Introduction to the problem

Solving a **PDE** means to find a function u such that

$$\mathcal{L}u = f$$

where \mathcal{L} is a differential operator and f is a source term.

The equation holds in a domain Ω and is completed by prescribing **boundary conditions** on $\partial\Omega$.

In most physical applications \mathcal{L} is a second-order operator

- Poisson equation: $\mathcal{L} = -\Delta$
- Heat equation: $\mathcal{L} = \frac{\partial}{\partial t} - \Delta$
- Wave equation: $\mathcal{L} = \frac{\partial^2}{\partial t^2} - c^2 \Delta$

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Weak formulation

Galerkin methods rely on a **weak formulation**

- Multiply by a test function v and integrate over the entire domain

$$-\int_{\Omega} (\Delta u) v d\Omega = \int_{\Omega} f v d\Omega$$

- Integrate by parts the left hand side

$$-\int_{\Omega} (\Delta u) v d\Omega = \int_{\Omega} \nabla u \cdot \nabla v d\Omega - \int_{\partial\Omega} \frac{\partial u}{\partial n} v ds$$

- Substitute and get the new expression

$$\int_{\Omega} \nabla u \cdot \nabla v d\Omega = \int_{\Omega} f v d\Omega + \int_{\partial\Omega} \frac{\partial u}{\partial n} v ds$$

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About the test function

The test function v is introduced to check whether the PDE is satisfied on average throughout the domain.

The problem becomes to find u such that

$$a(u, v) = F(v) \quad \forall v \in V$$

where

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v d\Omega \quad \text{is a } \underline{\text{bilinear form}}$$

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Benefits of the weak formulation

Strong formulation

$$u \in C^2(\Omega)$$

Holds pointwise in Ω

Derivatives exist classically

Weak formulation

$$u, v \in H^1(\Omega)^*$$

Holds on average on Ω

Derivatives exist in the distributional sense

In short: weak formulation requires **less regularity**

* $H^1(\Omega)$ is a **Sobolev space** of functions with square-integrable first derivatives:

$$w \in H^1(\Omega) = \left\{ w \in L^2(\Omega) \mid \nabla w \in L^2(\Omega)^d \right\}$$

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On boundary conditions

Another difference lies in the boundary condition prescription.



$v = 0$ on $\partial\Omega \Rightarrow$ cancels boundary term
 (no information available on $\frac{\partial u}{\partial n}$)

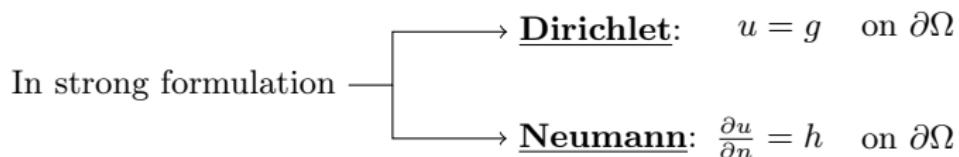
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$u = g$ enforced on $\partial\Omega$ (final solution)

$\frac{\partial u}{\partial n} = h$ naturally enters weak form

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Dirichlet becomes
essential condition

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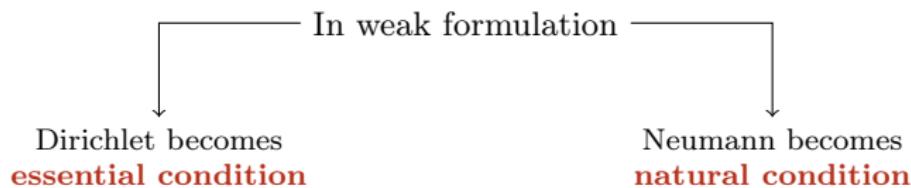
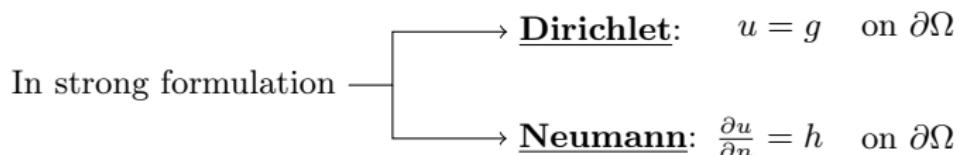
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Shape functions

Galerkin methods allow to find an approximate solution

$$u_h \in V_h \subset H^1(\Omega) \quad \text{where } V_h \text{ is a **finite-dimensional** space}$$

In this framework, the goal is to find u_h such that

$$a(u_h, v_h) = F(v_h) \quad \forall v_h \in V_h$$

A basis of function $\{\phi_i\}$ is chosen to express u_h and to use it as test:

$$u_h = \sum_{j=1}^N u_j \phi_j \implies a\left(\sum_{j=1}^N u_j \phi_j, \phi_i\right) = F(\phi_i) \quad \forall i = 1, \dots, N$$

Functions ϕ_i model the solution \longrightarrow **shape functions**

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Final expression

By linearity of $a(\cdot, \cdot)$, the problem reduces to a **finite linear system**:

$$\sum_{j=1}^N u_j a(\phi_j, \phi_i) = F(\phi_i) \quad \forall i = 1, \dots, N$$

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$$A\mathbf{u} = \mathbf{F}$$

where

$$A_{i,j} = a(\phi_j, \phi_i)$$

form the **stiffness matrix**

$$\mathbf{u} = (u_1, \dots, u_N)^T$$

is the **vector of unknowns**

$$\mathbf{F} = (F(\phi_1), \dots, F(\phi_N))^T$$

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Mesh discretization

FEM approach consists in the subdivision of the domain in a so-called **mesh**

This choice brings several advantages:

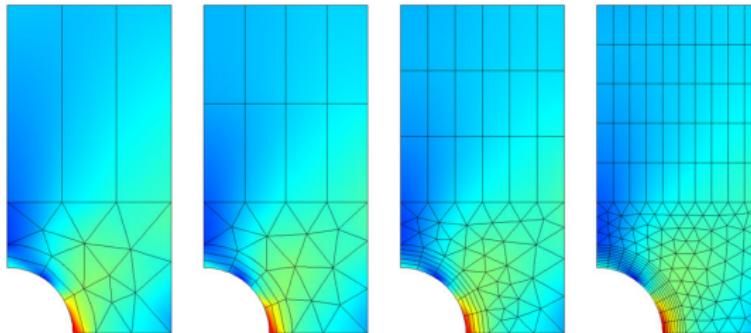
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- Better capture of **local effects**
- Possibility of **adaptive refinement**
- Natural construction of a **global solution**

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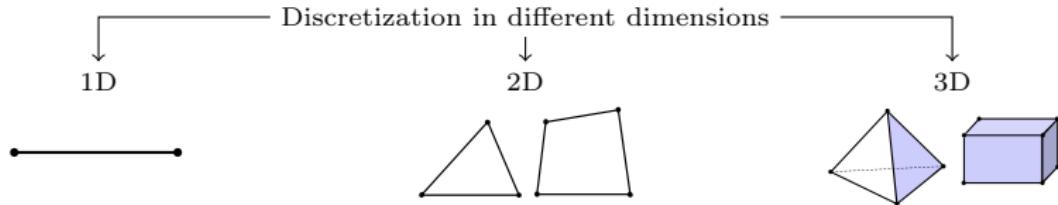
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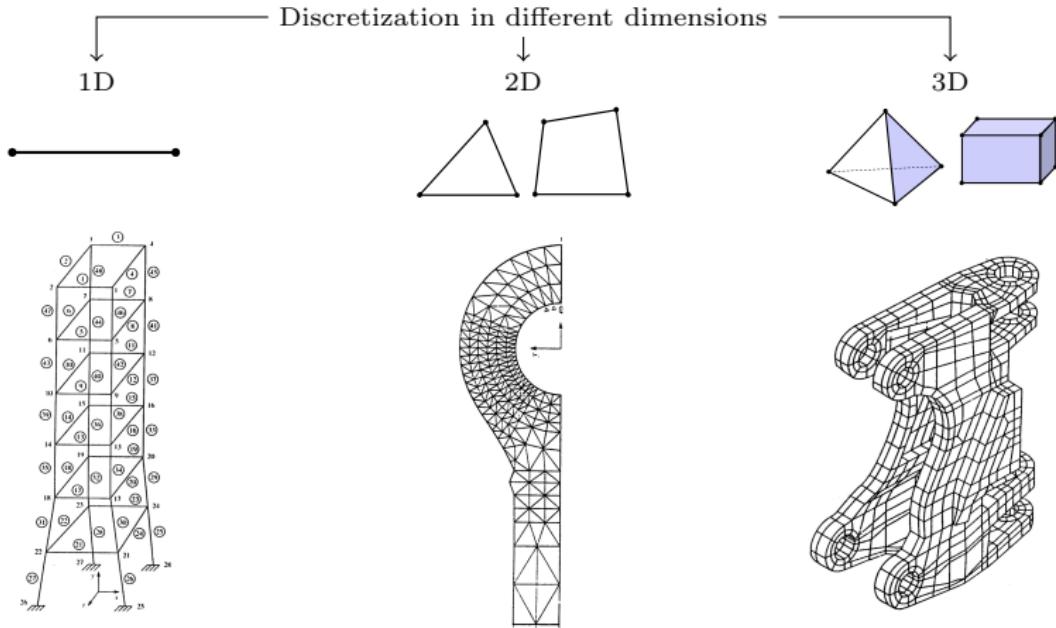
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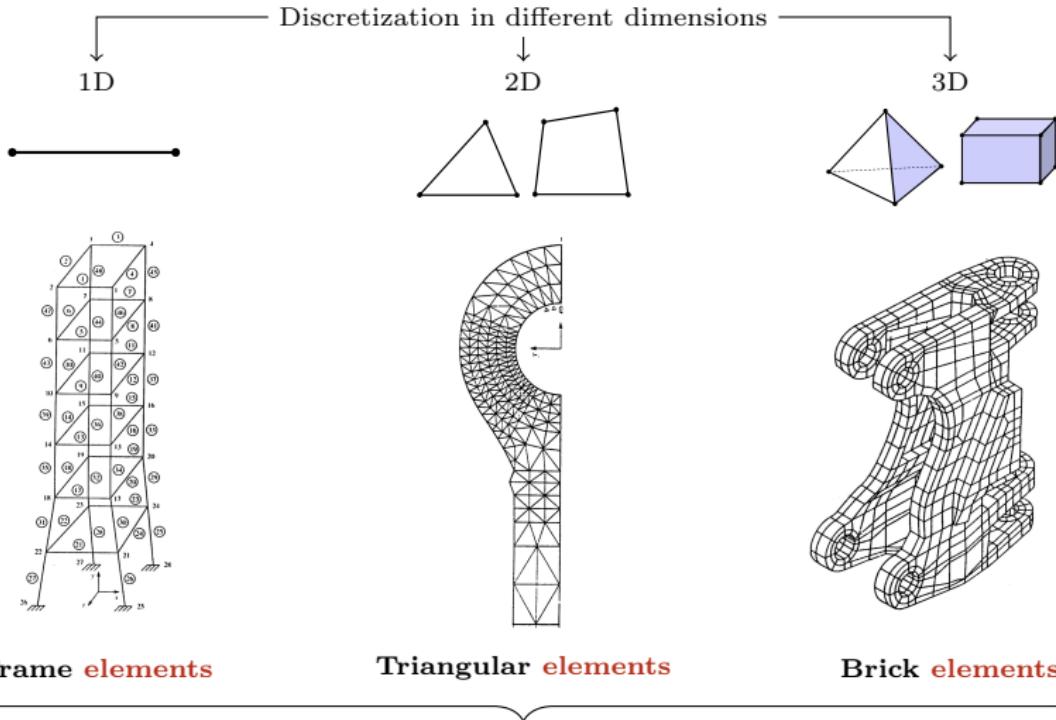
Elements



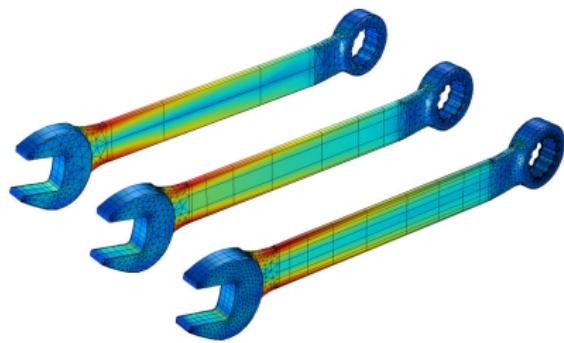
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Application examples

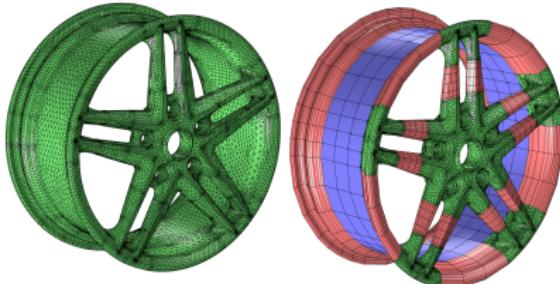


Manual mesh refinement of a wrench using different element types

Image from COMSOL Multiphysics Encyclopedia, "Finite Element Mesh Refinement", 21st of February 2017

Mesh of a wheel rim composed of tetrahedrons in green, bricks in blue and prisms in pink

Image from COMSOL Multiphysics Blog, "Meshing Your Geometry: When to Use the Various Element Types", Walter Frei, 4th of November 2013



Choise of the base

Mesh division into sub-domains



Choice of a **local basis functions**



Exploitation of compact support



- Leads to sparse matrices
- Allows local interpolation
- Enhances numerical stability
- Enables efficient parallelization

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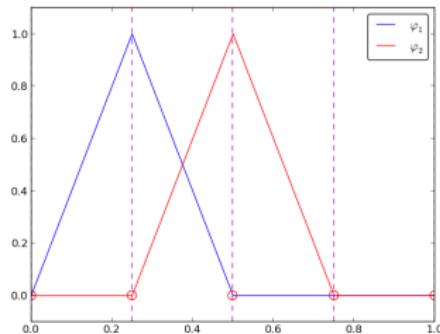


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FEniCS library

A leading software platform for finite element computations is **FEniCS**.

- Open-source and freely available
- Multi-language support (C++ and Python APIs)
- Parallel computing with MPI support

FEniCS package: $\left\{ \begin{array}{ll} \text{DOLFIN} & (\text{backend core engine and PETSc interface}) \\ \text{UFL} & (\text{symbolic language}) \\ \text{FIAT} & (\text{shape functions tabulator}) \\ \text{FFC} & (\text{C++ compiler for efficient local assembly}) \\ \text{MSHR} & (\text{mesh generator}) \end{array} \right.$

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A minimal FEniCS example: setup

Setup of a Poisson equation with Neumann boundary conditions in FEniCS:

- Generation of the mesh

```
domain = mesh.create_interval(MPI.COMM_WORLD, nx, [0.0, L])
```

- Definition of the finite element function space

```
V = functionspace(domain, ("Lagrange", 1))
```

- Definition of trial function and test function

```
u = ufl.TrialFunction(V)
v = ufl.TestFunction(V)
```

- Definition of the source term

```
f = fem.Constant(domain, default_scalar_type(-6))
```

A minimal FEniCS example: solution

Solving Poisson equation with Neumann boundary conditions in FEniCS:

- Weak formulation

```
a = ufl.dot(ufl.grad(u), ufl.grad(v)) * ufl.dx
F = f * v * ufl.dx
```

- Solution of the linear system

```
problem = LinearProblem(a, F,
                        petsc_option = {"ksp_type": "preonly",
                                      "pc_type" : "lu"
                                    })
u_h = problem.solve()
```

Approach to the classical wave equation

Our first goal is to approximate the solution of

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0 \quad \leftarrow \text{d'Alembert equation}$$



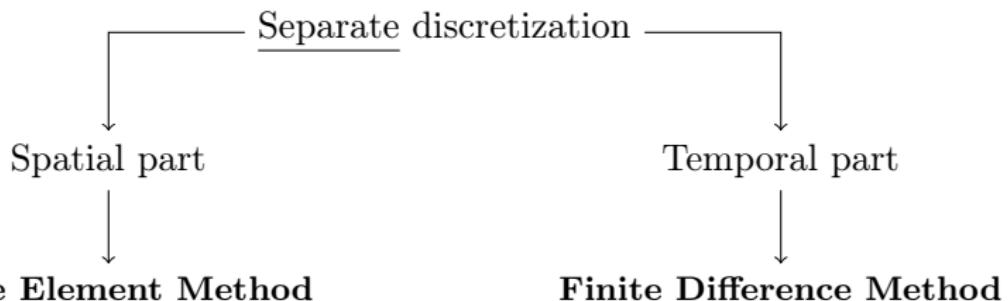
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$$\frac{\partial^2 u}{\partial t^2} \simeq \frac{u^{(n+1)} - 2u^{(n)} + u^{(n-1)}}{\Delta t^2}$$

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From PDE to ODEs

To do so, a **separable base** must be chosen:

$$u_h(x, t) = \sum_{j=1}^N u_j(t) \phi_j(x)$$

Managing the boundary term separately, the weak formulation goes as

$$\int_0^L \frac{\partial^2 u}{\partial t^2} v dx + c^2 \int_0^L \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} dx = 0 \quad \forall v \in H^1([0, L])$$



$$\sum_{j=1}^N \frac{d^2 u_j}{dt^2} \int_0^L \phi_j \phi_i dx + c^2 \sum_{j=1}^N u_j \int_0^L \frac{\partial \phi_j}{\partial x} \frac{\partial \phi_i}{\partial x} dx = 0 \quad \forall i = 1, \dots, N$$

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Matrix formulation

Let's define

$$M : M_{i,j} = \int_0^L \phi_j \phi_i dx \quad \leftarrow \text{Mass matrix}$$

$$A : A_{i,j} = \int_0^L \frac{\partial \phi_j}{\partial x} \frac{\partial \phi_i}{\partial x} dx \quad \leftarrow \text{Stiffness matrix}$$



$$M \frac{d^2 u}{dt^2} + c^2 A u = 0$$

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Time discretization

Let's apply **implicit central difference scheme**:

$$M \frac{\mathbf{u}^{(n+1)} - 2\mathbf{u}^{(n)} + \mathbf{u}^{(n-1)}}{\Delta t^2} + c^2 A \mathbf{u}^{(n+1)} = 0$$



$$\left(\frac{1}{\Delta t^2} M + c^2 A \right) \mathbf{u}^{(n+1)} = \frac{2}{\Delta t^2} M \mathbf{u}^{(n)} - \frac{1}{\Delta t^2} M \mathbf{u}^{(n-1)}$$

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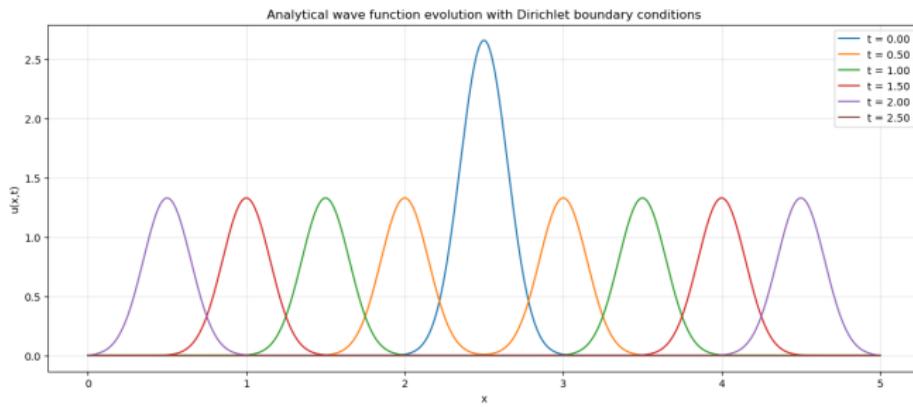
Analytical solutions

Solutions are known since 1747 due to d'Alembert himself.

- Dirichlet boundary conditions: $u(0, t) = u(L, t) = 0$

$$u(x, t) = \sum_{n=1}^{\infty} A_n \cos\left(\frac{n\pi}{L}ct\right) \sin\left(\frac{n\pi}{L}x\right)$$

with $A_n = \frac{2}{L} \int_0^L f(x) \sin\left(\frac{n\pi}{L}x\right) dx$.



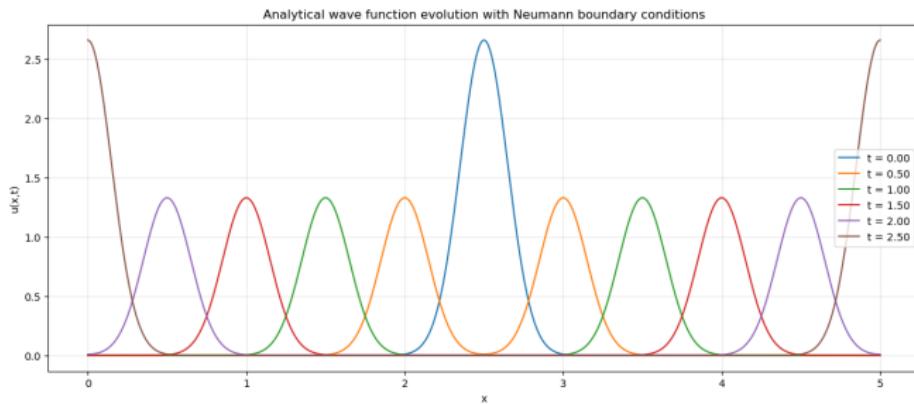
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- **Neumann** boundary conditions: $\frac{\partial u}{\partial x}\Big|_{x=0} = \frac{\partial u}{\partial x}\Big|_{x=L} = 0$

$$u(x, t) = A_0 + \sum_{n=1}^{\infty} A_n \cos\left(\frac{n\pi}{L}ct\right) \cos\left(\frac{n\pi}{L}x\right)$$

with $A_0 = \frac{1}{L} \int_0^L f(x)dx$, $A_n = \frac{2}{L} \int_0^L f(x) \cos\left(\frac{n\pi}{L}x\right) dx$.



Approximate solutions

The selection of discretization steps should* take into account

$$\text{CFL stability condition : } \frac{c\Delta t}{\Delta x} \lesssim 1$$

Choosing first-order Lagrange polynomials as $\{\phi_i\}$:

*While for implicit schemes it is only a recommendation, for explicit ones it is mandatory.

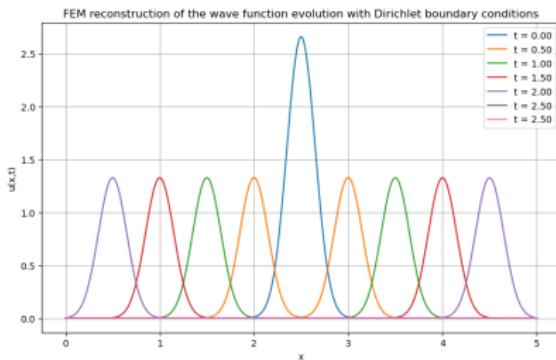
Approximate solutions

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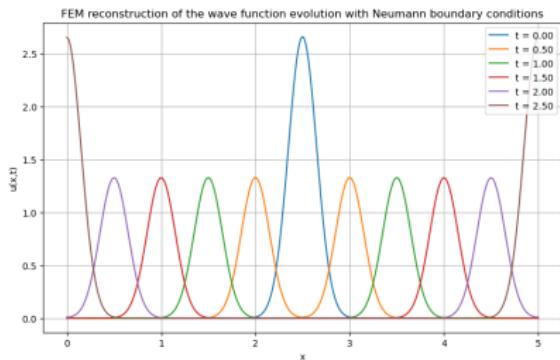
$$\text{CFL stability condition : } \frac{c\Delta t}{\Delta x} \lesssim 1$$

Choosing first-order Lagrange polynomials as $\{\phi_i\}$:

Dirichlet



Neumann



* While for implicit schemes it is only a recommendation, for explicit ones it is mandatory.

Energy loss

A strong indicator of numerical correctness is **energy conservation**.

$$\text{Energy: } E = \underbrace{\frac{T}{2c^2} \int_0^L \left(\frac{\partial u}{\partial t} \right)^2 dx}_{\text{Kinetic}} + \underbrace{\frac{T}{2} \int_0^L \left(\frac{\partial u}{\partial x} \right)^2 dx}_{\text{Potential}}$$

T is the *tension*, which can be arbitrarily set to 1.

Numerical energy decay is *independent* of the CFL number, being entirely caused by the **implicit scheme** itself.

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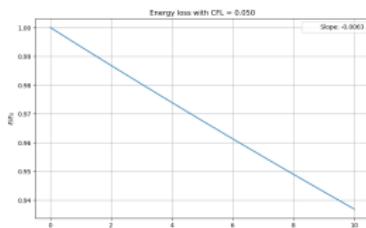
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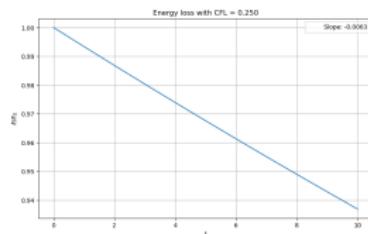
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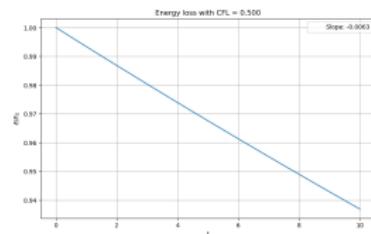
CFL = 0.05



CFL = 0.25



CFL = 0.50



Numerical energy decay is *independent* of the CFL number, being entirely caused by the **implicit scheme** itself.

What if $c = c(x)$?

If c is not constant, its square must be interpolated as the wave function:

$$c(2x) \longrightarrow c_h^2(x) = \sum_{k=1}^N c_k^{(2)} \psi_k(x)$$

Velocity must be included in the stiffness matrix A :

$$A_{i,j} = \int_0^L \left(\sum_{k=1}^N c_k^{(2)} \psi_k(x) \right) \frac{\partial \phi_j}{\partial x} \frac{\partial \phi_i}{\partial x} dx$$



$$M \frac{d^2 u}{dt^2} + A u = 0$$

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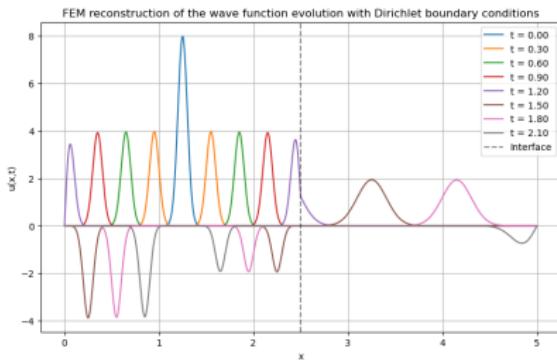
Piecewise constant velocity

One simple example is the **piecewise constant function**:

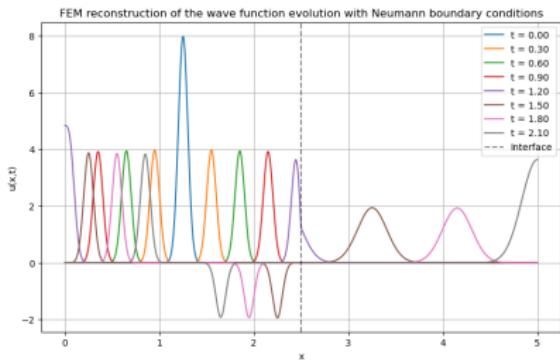
$$c(x) = \begin{cases} c_1 & x \leq x_0 \\ c_2 & x > x_0 \end{cases}$$

Placing initial pulse on the left with $c_1 = 1, c_2 = 3$:

Dirichlet



Neumann



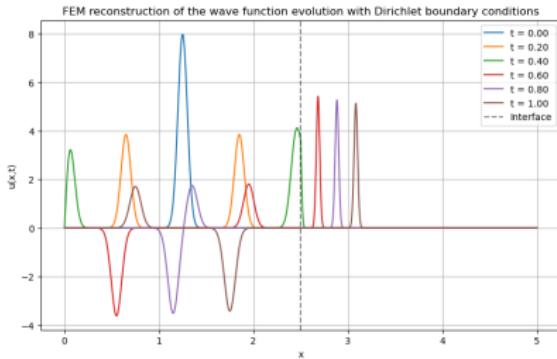
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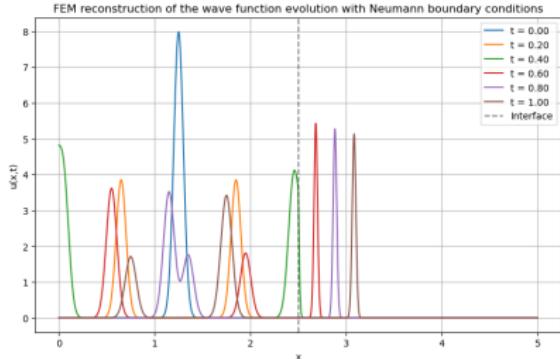
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Placing initial pulse on the left with $c_1 = 3, c_2 = 1$:

Dirichlet



Neumann



Fresnel coefficients

In this case, the analytical reference values are the **Fresnel coefficients**.

$$T = \frac{2c_1}{c_1 + c_2} \quad R = \frac{c_2 - c_1}{c_1 + c_2}$$

T and R are numerically evaluated as the ratio of the transmitted and reflected waves to the incident one.

Smaller velocity \rightarrow Smaller coefficient \rightarrow Higher sensitivity to numerical errors

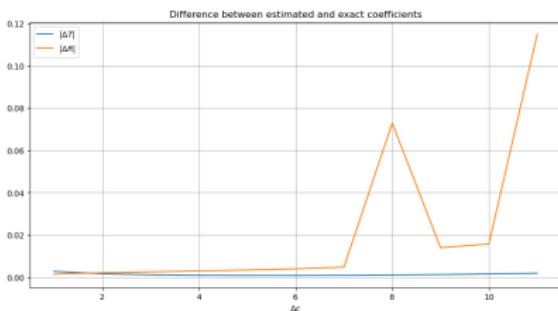
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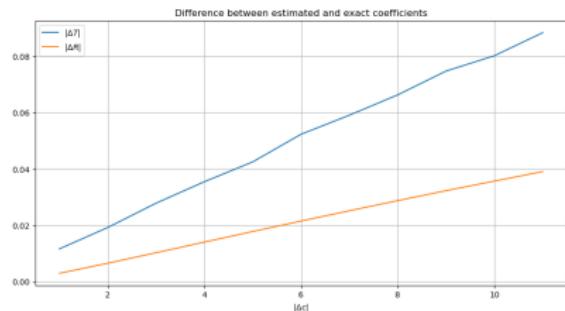
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$$c_1 < c_2$$



$$c_1 > c_2$$

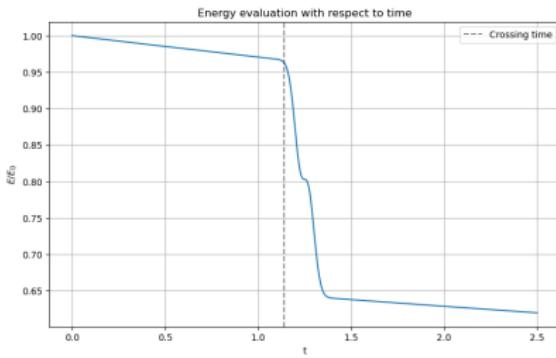


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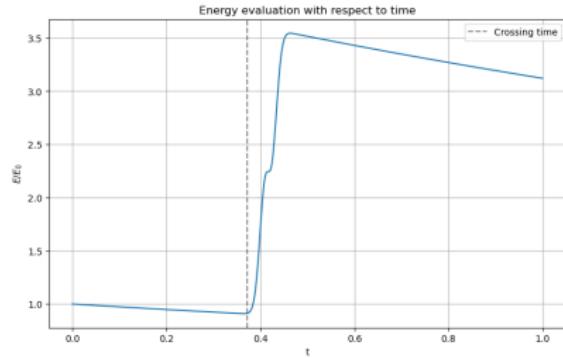
Energy variation

Right after the wave crosses the interface, a clear **non-conservation of energy** emerges.

$$c_1 = 1 \quad c_2 = 3$$



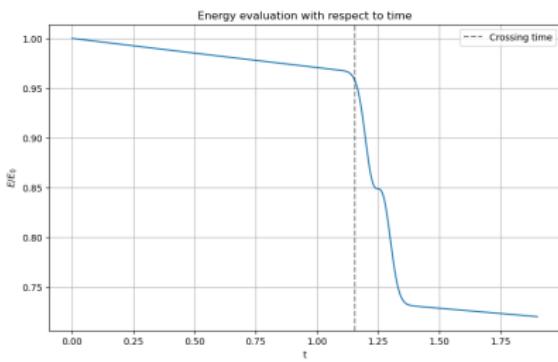
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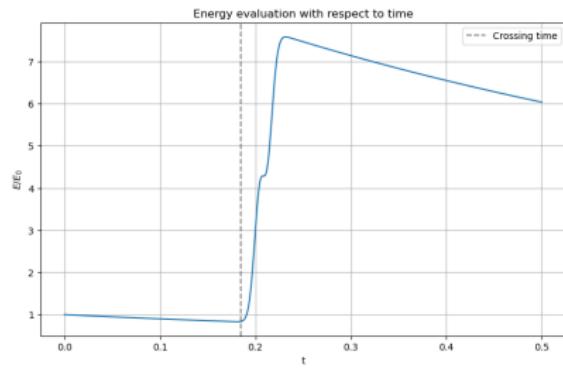
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Right after the wave crosses the interface, a clear **non-conservation of energy** emerges.

$$c_1 = 1 \quad c_2 = 6$$



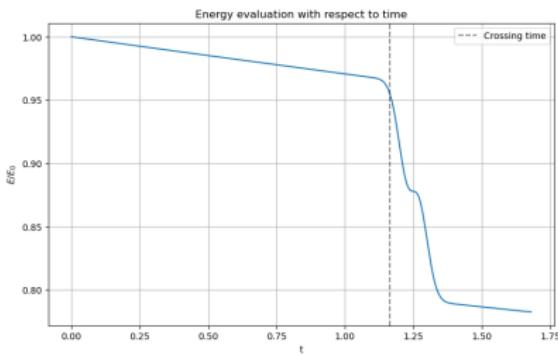
$$c_1 = 6 \quad c_2 = 1$$



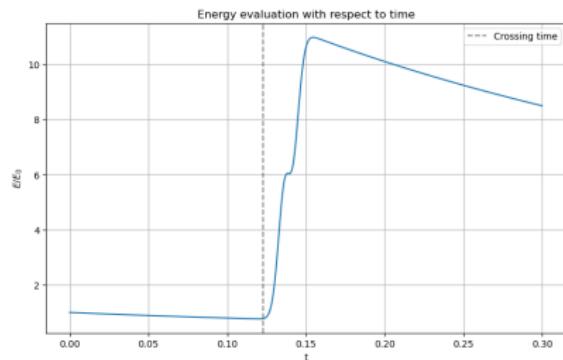
Energy variation

Right after the wave crosses the interface, a clear **non-conservation of energy** emerges.

$$c_1 = 1 \quad c_2 = 9$$

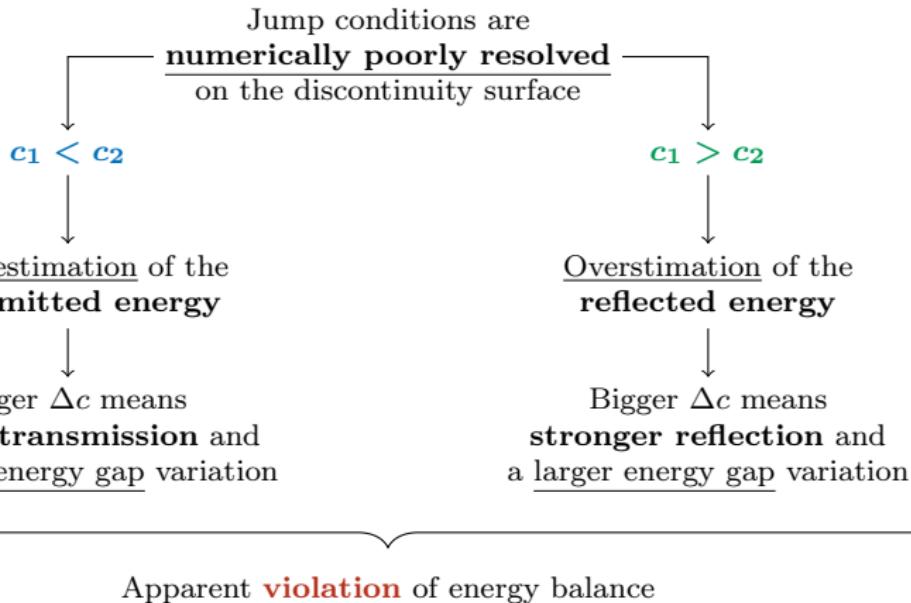


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Energy variation

Right after the wave crosses the interface, a clear **non-conservation of energy** emerges.



Approach to the Schrödinger equation

Moving in the quantum realm, our next goal is to approximate the solution of a **1D time-dependent Schrödinger equation**:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x, t)$$



$$\underbrace{i\hbar \sum_{j=1}^N \frac{d\psi_j}{dt} \int_{-L}^L \phi_j \phi_i dx}_{i\hbar M \frac{d\psi}{dt}} = \underbrace{\frac{\hbar^2}{2m} \sum_{j=1}^N \psi_j \int_{-L}^L \frac{\partial \phi_j}{\partial x} \frac{\partial \phi_i}{\partial x} dx}_{\frac{\hbar^2}{2m} A\psi} + \sum_{j=1}^N \psi_j \int_{-L}^L V \phi_j \phi_i dx$$

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Potential matrix

In the equation it appears a linear term.

We must then introduce a new matrix, that can be called **potential matrix**, which is nothing different than a **weighted mass matrix**:

$$V : V_{i,j} = \int_{\Omega} V(x) \phi_j(x) \phi_i(x) dx$$



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Application of the Crank-Nicholson method

In this case, the PDE is of first order in time.

The most suitable method to use is the **Crank-Nicholson** scheme:

$$M \frac{\psi^{(n+1)} - \psi^{(n)}}{\Delta t} = -\frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} A + V \right) \psi^{(n+1)} - \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} A + V \right) \psi^{(n)}$$



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How to handle imaginary part

The imaginary unit implies that the wavefunction is complex-valued.
 In order to work with standard real-valued FEM solvers, we apply a **real-imaginary splitting**:

$$\psi^{(i)} = \mathbf{u}^{(i)} + i\mathbf{w}^{(i)}$$

Setting $\alpha = \frac{\Delta t}{2\hbar}$ and $H = \frac{\hbar^2}{2m}A + V$:

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Block matrix formulation

Concatenating real and imaginary components in a single vector, the final expression is

$$\begin{pmatrix} M & -\alpha H \\ \alpha H & M \end{pmatrix} \begin{pmatrix} \mathbf{u}^{(n+1)} \\ \mathbf{w}^{(n+1)} \end{pmatrix} = \begin{pmatrix} M & \alpha H \\ -\alpha H & M \end{pmatrix} \begin{pmatrix} \mathbf{u}^{(n)} \\ \mathbf{w}^{(n)} \end{pmatrix}$$

As before, the problem is recast as a **linear system of equations**.

Free particle scenario

If $V(x) = 0$, the solution of the Schrödinger equation describes a system called **free particle**.

A gaussian $\mathcal{G}(x|x_0, \sigma_0)$ can be chosen as *initial wave packet*:

$$\psi(x, 0) = (\pi\sigma_0^2)^{-\frac{1}{4}} e^{-\frac{(x-x_0)^2}{2\sigma_0^2} + ik_0 x}$$

We know the analytical solution of the equation:

$$\boxed{\psi(x, t) = \frac{1}{\sigma_t \sqrt{\pi}} e^{-\frac{(x-x_0 - \frac{\hbar k_0}{m} t)^2}{\sigma_t^2}} \quad \text{where } \sigma_t = \sigma_0 \sqrt{1 + \left(\frac{\hbar t}{m \sigma_0^2}\right)^2}}$$

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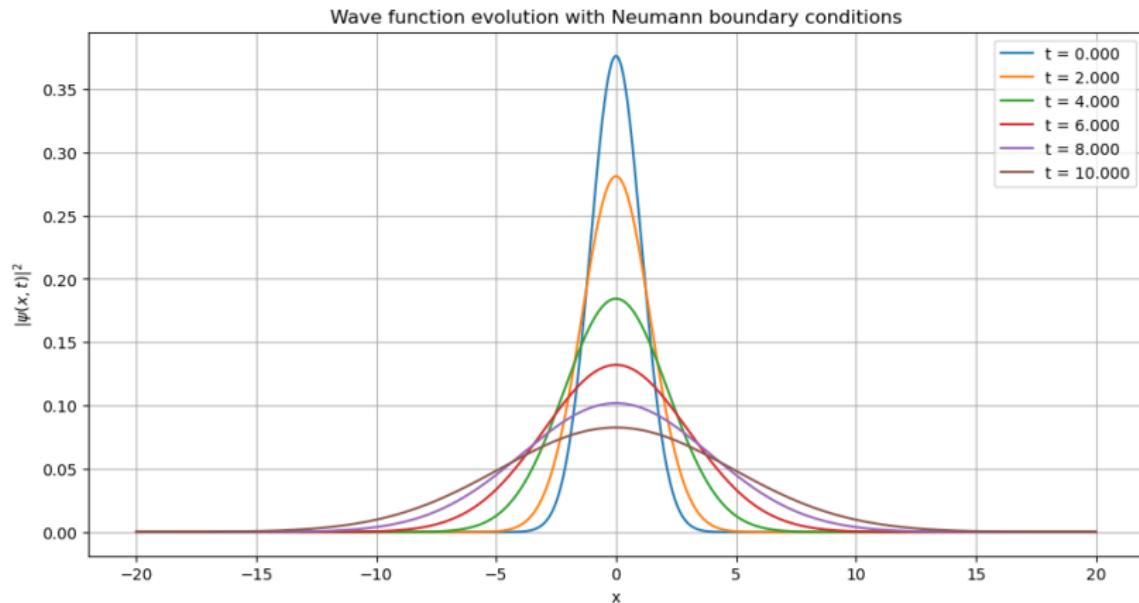
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Numerical simulation

Numerical simulation using FEM confirms the theoretical predictions.



Ballistic spreading

The numerical σ follows the same **ballistic behaviour** up until the time when the wavefunction reaches the boundary.

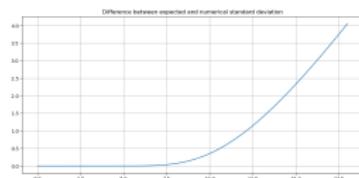
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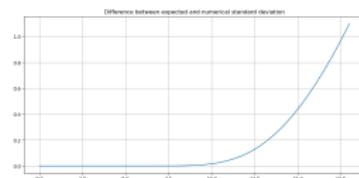
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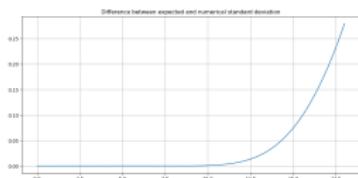
$$\sigma_0 = 0.10$$



$$\sigma_0 = 0.15$$



$$\sigma_0 = 0.20$$



Smaller error with larger σ_0 at equal times

Kronig-Penney model

The introduction of a **periodic potential** leads to what is called a **Kronig-Penney-like model**, which is used to describe electrons in a crystal lattice.

Bloch's theorem states that solutions to the Schrödinger equation in a periodic potential can be expressed as *plane waves* modulated by *periodic functions* $u(x)$ with the same periodicity as the crystal:

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Bloch waves

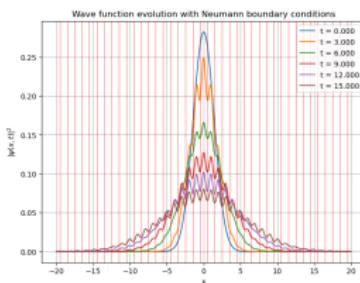
A periodic potential $V(x) = V_0 \cos\left(\frac{2\pi}{a}x\right)$ couples plane waves which differ of multiples of $\frac{2\pi}{a}$, and the resulting superpositions form the **Bloch waves**.

Projection onto periodic plane waves

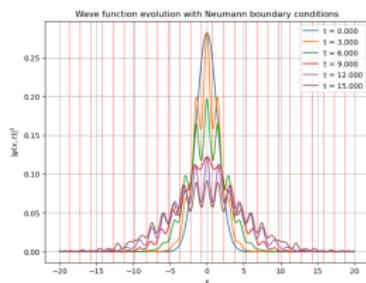


Formation of **lattice harmonics**

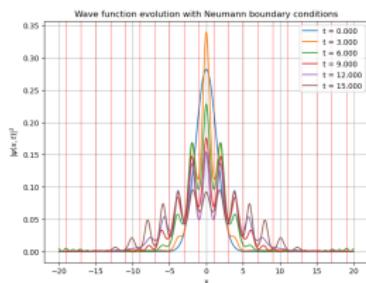
$$a = 1.0$$



$$a = 1.5$$



$$a = 2.0$$



Effective mass

With the periodic potential, the allowed energies are no longer continuous, but split into separate **bands**, each associated with different values of the *crystal momentum* k .

Taylor expansion around k_0 :

$$E(k) = E(k_0) + \frac{dE}{dk} \Big|_{k_0} (k - k_0) + \frac{1}{2} \frac{d^2E}{dk^2} \Big|_{k_0} (k - k_0)^2 + \dots$$

In the lowest bound, $k_0 = 0$ is the *minimum*:

$$E(k) \simeq E_0 + \frac{1}{2} \frac{d^2E}{dk^2} \Big|_{k=0} k^2$$

Comparing with the energy of a free particle, an **effective mass** can be found:

$$E(k) = E_0 + \frac{\hbar^2 k^2}{2m^*} \implies m^* = \hbar^2 \left(\frac{d^2E}{dk^2} \Big|_{k=0} \right)^{-1}$$

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Comparing with the energy of a free particle, an **effective mass** can be found:

$$E(k) = E_0 + \frac{\hbar^2 k^2}{2m^*} \implies m^* = \hbar^2 \left(\frac{d^2 E}{dk^2} \Big|_{k=0} \right)^{-1}$$

Effective mass

With the periodic potential, the allowed energies are no longer continuous, but split into separate **bands**, each associated with different values of the *crystal momentum* k .

Taylor expansion around k_0 :

$$E(k) = E(k_0) + \frac{dE}{dk} \Big|_{k_0} (k - k_0) + \frac{1}{2} \frac{d^2 E}{dk^2} \Big|_{k_0} (k - k_0)^2 + \dots$$

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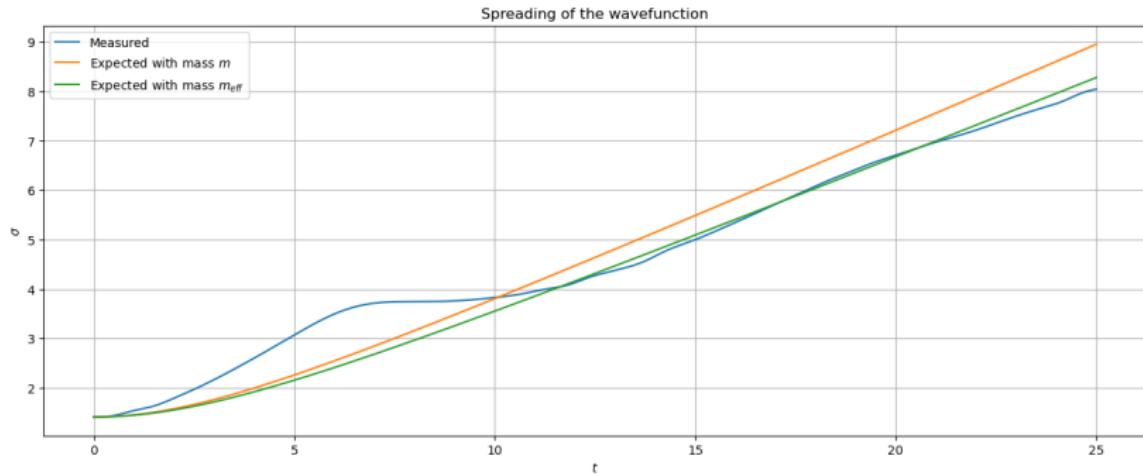
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Sub-ballistic spreading

Around the *minimum of a band*, a quantum system in a periodic lattice behaves like a free particle with an effective mass m^* .

Since $\sigma \propto \frac{1}{m}$, a slower spreading is expected for a periodic lattice where $m^* > m$, due to the **parabolic approximation** of the band energy.



Addition of a linear term

The mean value, on the contrary, does not change.

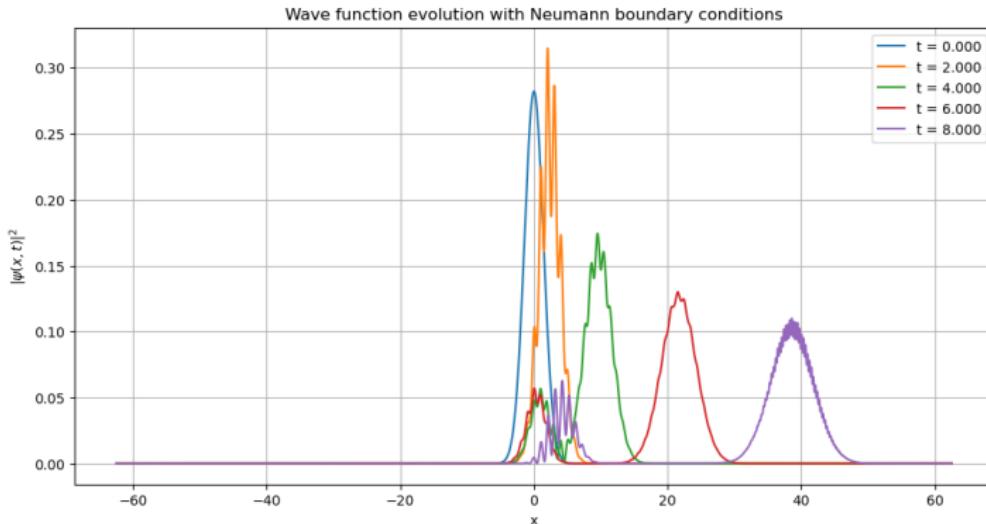
In order to induce a *net drift*, we must add a linear potential
 $V(x) = Fx$.

The plot shows how dispersion cases interference effects to gradually *fade*.

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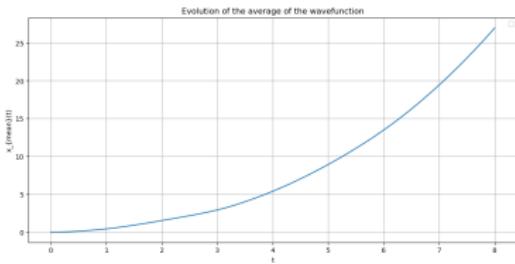
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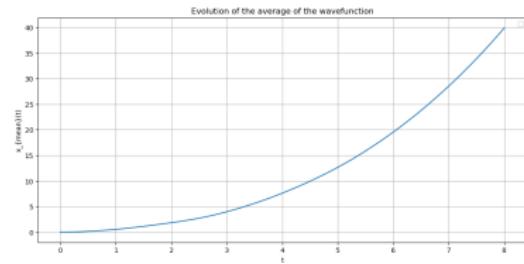


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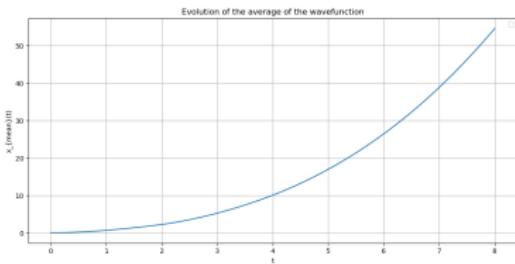
Average shift



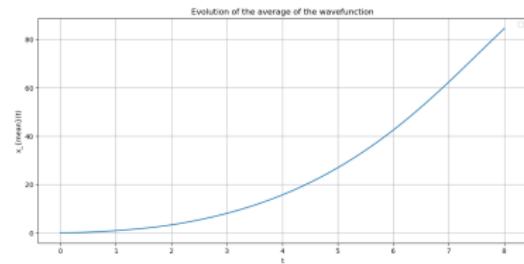
$$V_0 = 1.00, F = 1.00$$



$$V_0 = 1.00, F = 1.25$$



$$V_0 = 1.00, F = 1.50$$



$$V_0 = 1.00, F = 2.00$$

Conclusions

Some final considerations:

- FEM provides a suitable approach for **second-order PDEs**
- Even though it has been used for very simple domains, in principle it can be applied to very **complex geometries**
- To handle time evolution, FEM must be coupled with **finite difference schemes** or other temporal integration methods
- The choice of spatial mesh and time step must satisfy some **stability and accuracy criteria** (like CFL condition or norm conservation)
- FEM allows easy incorporation of **boundary conditions**

In summary, our examples show that FEM is a very **robust** and **versatile** tool for spatial discretization, but time evolution requires appropriate temporal schemes.

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Thank you for your attention!