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

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Numerical methods for differential equations

Ordinary Differential Equations

- Euler Method
- Crank-Nicolson Method
- Trotter-Suzuki Formula

Euler Method and Crank-Nicolson Method: **Runge-Kutta**

Partial Differential Equations

- Finite Difference Method
- Finite Volume Method
- Galerkin methods
  - Spectral Method
  - Finite Element Method

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Runge-**K**utta

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- **F**inite **V**olume **M**ethod
- Galerkin methods
  - Spectral Method
  - $\boxed{\text{Finite Element Method}}$

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

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

where

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

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Benefits of the weak formulation

Strong formulation	Weak formulation
$u \in C^2(\Omega)$	$u, v \in H^1(\Omega)^*$
Holds pointwise in Ω	Holds on average on Ω
Derivatives exist classically	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.

In strong formulation

- **Dirichlet**: $u = g \quad \text{on } \partial\Omega$
- **Neumann**: $\frac{\partial u}{\partial n} = h \quad \text{on } \partial\Omega$

In weak formulation

Dirichlet becomes **essential condition**	Neumann becomes **natural condition**
$\boldsymbol{v} = \mathbf{0}$ on $\partial\Omega \Rightarrow$ cancels boundary term (no information available on $\frac{\partial u}{\partial n}$)	$\boldsymbol{v}$ **free** on $\partial\Omega$
$\boldsymbol{u} = \boldsymbol{g}$ enforced on $\partial\Omega$ (final solution)	$\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{n}} = \boldsymbol{h}$ naturally enters weak form

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Shape functions

Galerkin methods allow to find an approximate solution

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

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

$$\boxed{a\left(u_h, v_h\right) = F\left(v_h\right) \qquad \forall v_h \in V_h}$$

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

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

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**:

$$\sum_{j=1}^{N} u_j a\left(\phi_j, \phi_i\right) = F\left(\phi_i\right) \qquad \forall i = 1, \ldots, N$$

$$\Downarrow$$

$$\boxed{A\boldsymbol{u} = \boldsymbol{F}}$$

where

$$A_{i,j} = a\left(\phi_j, \phi_i\right) \qquad \text{form the } \textbf{stiffness matrix}$$

$$\boldsymbol{u} = \left(u_1, \ldots, u_N\right)^T \qquad \text{is the } \textbf{vector of unknowns}$$

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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:

- Good approximation of **complex geometries**
- Better capture of **local effects**
- Possibility of **adaptive refinement**
- Natural construction of a **global solution**

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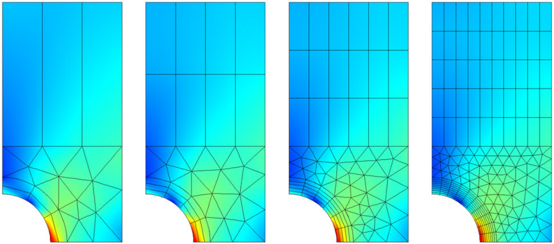
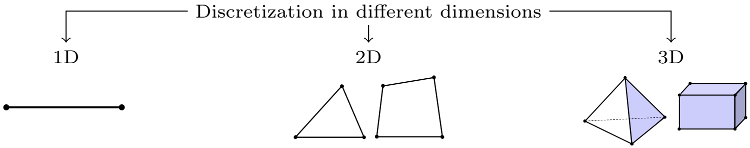


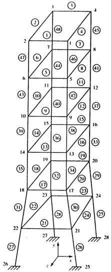
Elements



Elements

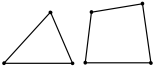
Discretization in different dimensions

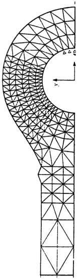
1D



Frame elements

2D





Triangular elements

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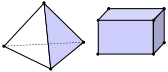

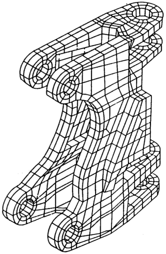

Brick elements

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Discretization in different dimensions

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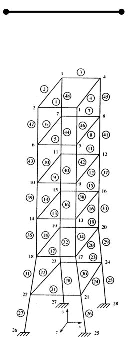

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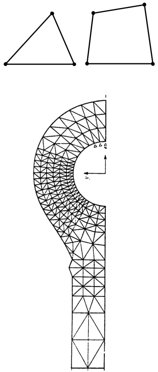

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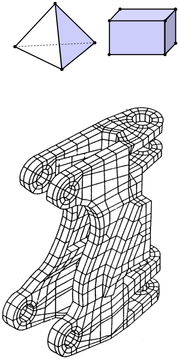
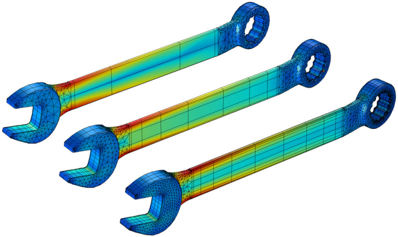


Brick elements

Finite Element Method

Application examples

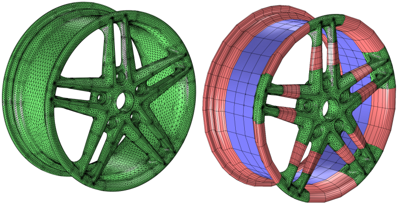


Manual mesh refinement of a wrench using different element types

Image from COMSOL Multiplysics Cyclopedia, ''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 Multiplysics 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**

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Exploitation of **compact support**

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

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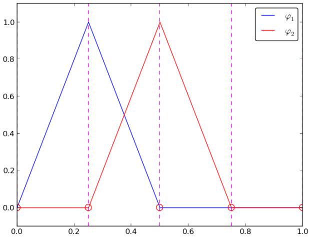

FEniCS library

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:

DOLFIN	(backend core engine and PETSc interface)
UFL	(symbolic language)
FIAT	(shape functions tabulator)
FFC	(C++ compiler for efficient local assembly)
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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()
```

Title

Our first goal is to approximate the solution of

$$\boxed{\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0} \longleftarrow \textbf{d'Alembert equation}$$

Equation is **separable**

Spatial part

$$-c^2 \int_0^L \frac{\partial^2 u}{\partial x^2} v dx =$$

Temporal part

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