Lecture 02 – Introduction to the Finite Element Method

... and some FEniCSx basics

1 Partial Differential Equations (PDEs)

Some PDE examples in a table:

Example Equation	Remark
$-\nabla \cdot (k\nabla u) = f$, temperature $u : \Omega \to \mathbb{R}$	Steady-state heat conduction, elliptic
$\frac{\partial u}{\partial t} - \nabla \cdot (k\nabla u) = f$	Transient heat conduction, parabolic
$\frac{\partial^2 u}{\partial t^2} - \mathrm{c}^2\nabla^2 u = 0$	Wave propagation, hyperbolic
$-\nabla \cdot (k\nabla u) + R(u) = f$, concentration $c : \Omega \to \mathbb{R}$, $R(u) = u(1-u)$ (e.g.)	Reaction-diffusion

1.1 Notation

For simplicity, we wrote PDEs in vector form, but they can also be expressed in component, e.g.

$$-\nabla \cdot (k\nabla u) = -\partial_x(k\partial_x u) - \partial_y(k\partial_y u) - \partial_z(k\partial_z u).$$

Other helpful differential operators include:

- Gradient: $\nabla u = \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial u}{\partial z}\right)$
- Divergence: $\nabla \cdot \mathbf{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}$ with $\mathbf{v} = (v_x, v_y, v_z)$
- Laplacian: $\Delta u = \nabla^2 u = \nabla \cdot \nabla u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$
- Rotation: $\nabla \times \mathbf{v} = \left(\frac{\partial v_z}{\partial y} - \frac{\partial v_y}{\partial z}, \frac{\partial v_x}{\partial z} - \frac{\partial v_z}{\partial x}, \frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y}\right)$

1.2 Boundary-value-problems (BVPs)

- Domain Ω with boundary Γ, the domain Ω is where the PDE holds. (Mathematically, a domain is an open, non-empty, connected subset of $\mathbb{R}^n$ (e.g., a 2D region or 3D volume), and the boundary is its edge)
- $\Gamma = \partial\Omega$ is where we specify boundary conditions, n is the outward normal vector on Γ.

Boundary conditions:

- Dirichlet: $u = u_D$ on Γ_D (specify value of u)
- Neumann: $-k\nabla u \cdot n = g_N$ on Γ_N (specify flux across boundary)
- Robin: $\alpha u + \beta(-k\nabla u \cdot n) = g_R$ on Γ_R (combination of value and flux)

A BVP:

$$\begin{cases} -\nabla \cdot (k\nabla u) = f & \text{in } \Omega, \\ u = u_D & \text{on } \Gamma_D, \\ -k\nabla u \cdot n = g_N & \text{on } \Gamma_N. \end{cases}$$

1.3 Exact solution

For some simpler BVPs, we can find an exact solution analytically.

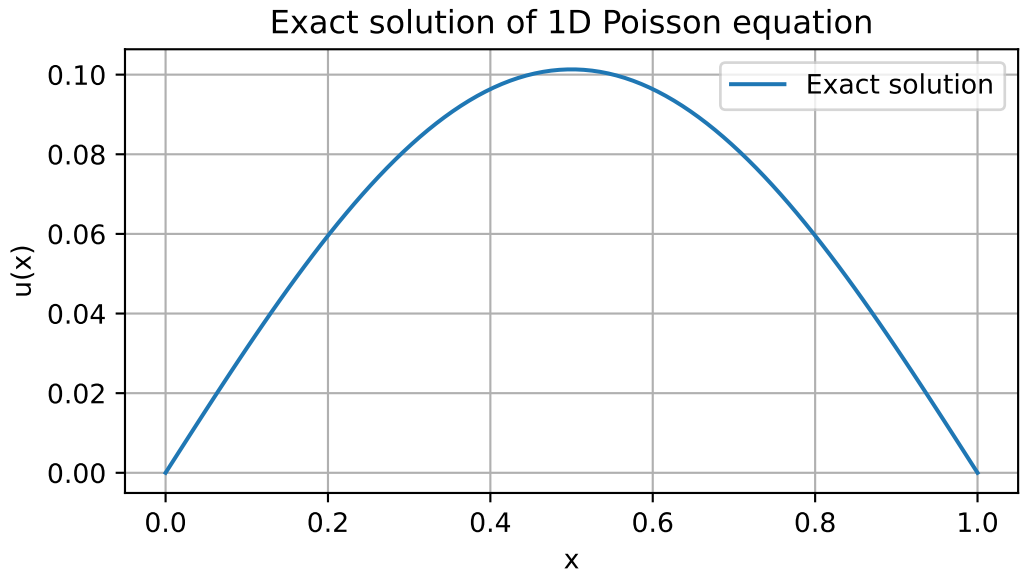
$$-\partial_x(k\partial_x u) = f(x) \quad \text{on } (0,1), \qquad u(0) = u(1) = 0.$$

with constant $k \in \mathbb{R}, k \neq 0$ and $f = \sin(\pi x)$ has exact solution:

$$u(x) = \tfrac{\sin(\pi x)}{k\pi^2}.$$

Since $\partial_x(k\partial_x u) = \partial_x\left(k\tfrac{\pi\cos(\pi x)}{k\pi^2}\right) = -\sin(\pi x)$, and the BCs are satisfied.

```
import numpy as np
import matplotlib.pyplot as plt
x = np.linspace(0, 1, 100)
k = 1.0
u = np.sin(np.pi * x) / (k * np.pi**2)
plt.plot(x, u, label='Exact solution')
plt.xlabel('x')
plt.ylabel('u(x)')
plt.title('Exact solution of 1D Poisson equation')
# change size
plt.gcf().set_size_inches(6, 3)
plt.grid(); plt.legend(); plt.show()
```



1.4 More complex domains

- For structured domains, the finite difference method (see exercise) can sometimes help.
- However, for more complex domains (e.g., with holes, curved boundaries), we need a more flexible method.

Finite element method (FEM): Can handle complex domains, unstructured meshes, and variable coefficients.

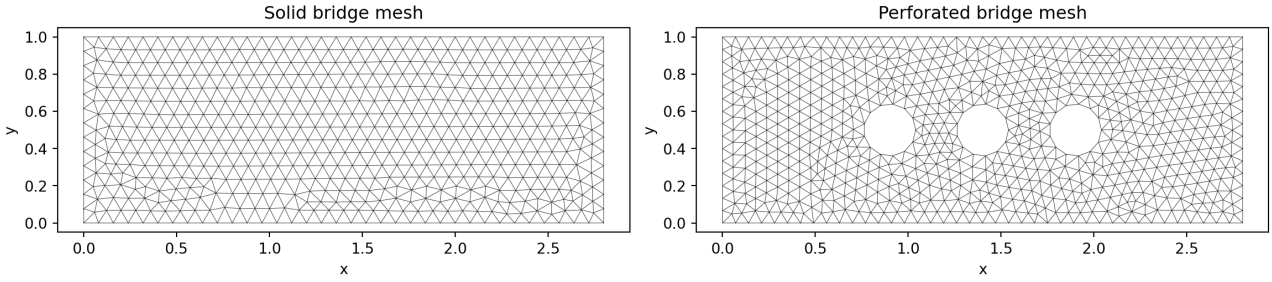


Figure 1: Mesh example

> **Note**
>
> The starting point for FEM is a *weak* (variational) formulation of the PDE.

2 Weak forms

For a given PDE (strong form), e.g., the Poisson equation with mixed BCs:

$$-\nabla \cdot (k\nabla u) = f \quad \text{in } \Omega, \qquad u = u_D \text{ on } \Gamma_D, \qquad -k\nabla u \cdot n = g_N \text{ on } \Gamma_N$$

1. multiply by a test function v and integrate over Ω to get the weak form:

$$\int_\Omega -\nabla \cdot (k\nabla u) v \, dx = \int_\Omega f v \, dx.$$

2. Apply integration by parts to move derivatives from u to v:

$$\int_\Omega k\nabla u \cdot \nabla v \, dx - \int_{\Gamma_N} (k\nabla u \cdot n) \, v \, ds = \int_\Omega f v \, dx$$

3. Insertion of Neumann BC:

$$\int_\Omega k\nabla u \cdot \nabla v \, dx = \int_\Omega f v \, dx + \int_{\Gamma_N} g_N v \, ds.$$

2.1 Variational problem

- Define trial space V and test space V_0
  - Sobolev space $H^1(\Omega)$ include functions with square-integrable derivatives, i.e., $H^1(\Omega) = \{w \in L^2(\Omega) \,|\, \nabla w \in (L^2(\Omega))^d\}$ meaning w and its gradient are square-integrable, i.e., $\int_\Omega |w|^2 \, dx < \infty$ and $\int_\Omega |\nabla w|^2 \, dx < \infty$.

$$V = \{w \in H^1(\Omega) \,|\, w = u_D \text{ on } \Gamma_D\}, \qquad V_0 = \{w \in H^1(\Omega) \,|\, w = 0 \text{ on } \Gamma_D\}.$$

Resulting problem: Find $u \in V$ such that

$$a(u, v) = L(v) \quad \forall v \in V_0,$$

with a form $a : V \times V_0 \to \mathbb{R}$ and a linear form $L : V_0 \to \mathbb{R}$ defined as

$$a(u, v) = \int_\Omega k \nabla u \cdot \nabla v \, dx, \qquad L(v) = \int_\Omega f v \, dx + \int_{\Gamma_N} g_N v \, ds.$$

2.2 The energy viewpoint (homogeneous BCs, $k = 1$)

- Start from an energy functional: $E(u) = \frac{1}{2} \int_\Omega |\nabla u|^2 \, dx - \int_\Omega f u \, dx$.
- Gateaux derivative: $E'(u; v) = \lim_{\epsilon \to 0} \frac{E(u+\epsilon v) - E(u)}{\epsilon} = \int_\Omega \nabla u \cdot \nabla v \, dx - \int_\Omega f v \, dx$.
- Energy minimization (calculus of variations): $\min_{u \in H_0^1(\Omega)} E(u)$ leads to $E'(u; v) = 0$ for all "direction" $v \in V_0$ as the first-order optimality condition, which is exactly the weak form.

$$\begin{aligned} E'(u; v) &= \lim_{\epsilon \to 0} \frac{E(u + \epsilon v) - E(u)}{\epsilon} \\ &= \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left(\frac{1}{2} \int_\Omega \nabla(u + \epsilon v) \cdot \nabla(u + \epsilon v) \, dx - \int_\Omega f(u + \epsilon v) \, dx - \left(\int_\Omega |\nabla u|^2 \, dx - \int_\Omega f u \, dx \right) \right) \\ &= \int_\Omega \nabla u \cdot \nabla v \, dx - \int_\Omega f v \, dx \stackrel{!}{=} 0 \quad \forall v \in V_0. \end{aligned}$$

See [Brezzi & Fortin, 1991]

2.3 Implementation: Galerkin

- Start from a variational form: find $u \in V_0$ such that $a(u, v) = L(v) \forall v \in V_0$.
- Galerkin: choose $V_h \subset V_0$ and solve $a(u_h, v_h) = L(v_h) \quad \forall v_h \in V_h$.
- Therefore, $u_h = \sum_{j=1}^N U_j \phi_j$ with basis functions $\{\phi_j\}$ of V_h and unknown coefficients U_j.
- Inseration into the variational form and testing with basis ϕ_i leads to:

$$\sum_{j=1}^N U_j a(\phi_j, \phi_i) = L(\phi_i) \quad \forall i = 1, \ldots, N,$$

2.4 Coefficient equation

Linear system of equations:

$$AU = b \quad \Leftrightarrow \quad \sum_{j=1}^{N} A_{ij} U_j = b_i \quad \forall i = 1, \dots, N,$$

with $A_{ij} = a(\phi_j, \phi_i) = \int_\Omega \nabla\phi_j \cdot \nabla\phi_i \, dx$ and $b_i = L(\phi_i) = \int_\Omega f\phi_i \, dx$.

P1 (linear) elements have 3 nodes per triangle (vertices)

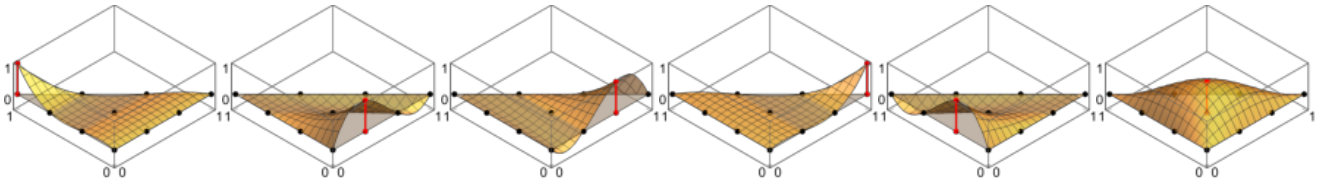
(a) P1 Lagrange 1

(a) P1 Lagrange 2

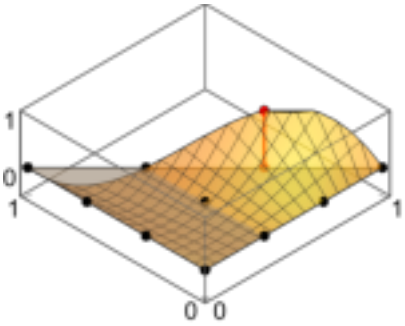
(a) P1 Lagrange 2

- Implementation can be annoying: See, e.g., these notes

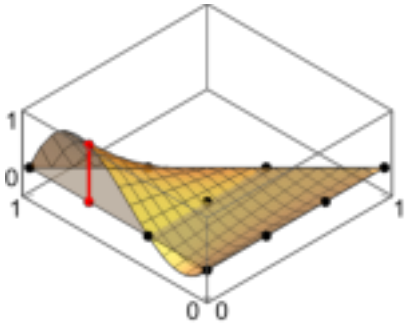
P3 Lagrange elements (cubic polynomials) have more nodes and higher-order basis functions, leading to better accuracy but also larger linear systems.



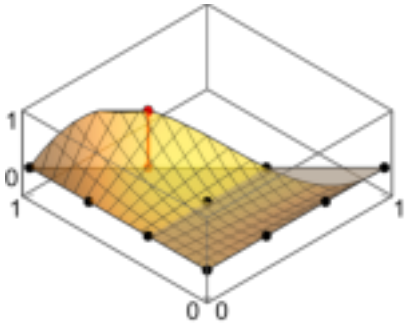
(a) P3 Lagrange 1 (a) P3 Lagrange 2 (a) P3 Lagrange 3 (a) P3 Lagrange 4 (a) P3 Lagrange 5 (a) P3 Lagrange 6



(a) P3 Lagrange 7



(a) P3 Lagrange 8



(a) P3 Lagrange 9

3 FEniCS framework

- FEniCS automates the whole process: from mesh generation, function space construction, variational form definition, assembly, to solving linear systems.
- You can focus on the model (weak form)
- Software Components (c.f. Lambert's M.Sc. thesis):
  - UFL: The Unified Form Language is a domain-specific language to formulate problems. It serves as the input for the form compiler.
  - FFCX: The FEniCS Form Compiler automatically generates DOLFIN code from a given variational form. The goal of a form compileris to use a well-tested compiler, performing automated code generation tasks, in order to improve the correctness of the resulting code.

– BASIX/FIAT: The FInite element Automatic Tabulator enables the automatic computation of basis functions for nearly arbitrary finite elements.

3.1 Elements and forms

- FEniCS supports a wide range of finite elements (Lagrange, Raviart–Thomas, Nédélec, etc.), see BASIX
- UFL allows to express variational forms (linear, nonlinear, time-dependent), for example:

```
u = ufl.TrialFunction(V)
v = ufl.TestFunction(V)
a = k * ufl.dot(ufl.grad(u), ufl.grad(v)) * ufl.dx
L = f * v * ufl.dx + g_N * v * ulf.ds
```

Other operators from UFL: `ufl.div`, `ufl.curl`, `ufl.cross`, `ufl.inner`, `ufl.outer`, etc.

Einstein summation convention is supported: `Dx(v, i)*Dx(w, i)` means $\sum_{i=1}^{d} \frac{\partial v}{\partial x_i} \frac{\partial w}{\partial x_i}$.

3.2 Algorithmic Workflow

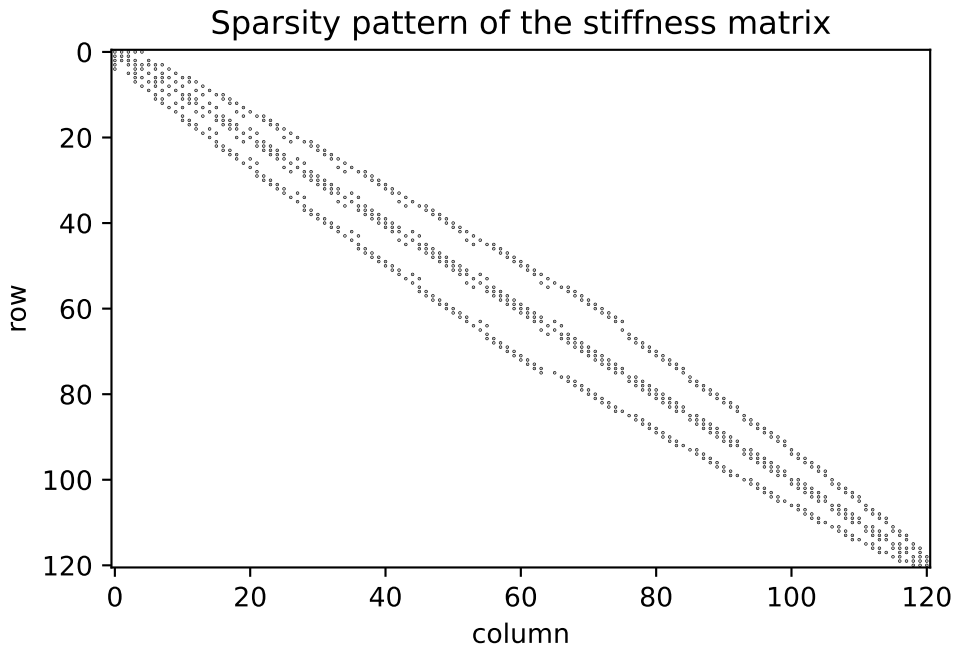
1. Generate (or load) mesh $\mathcal{T}_h$ and boundary markers.
2. Build finite element space V_h.
3. Define variational forms $a(\cdot,\cdot), L(\cdot)$.
4. Assemble sparse matrix/vector.
5. Apply boundary conditions.
6. Solve with direct or iterative solver.
7. [Estimate error / refine mesh postprocess]

3.3 Minimal FEniCSx Example (Unit Square)

```
from mpi4py import MPI
from petsc4py import PETSc
import inspect
import numpy as np
import ufl
from dolfinx import fem, mesh
from dolfinx.fem.petsc import LinearProblem

# Mesh and function space
msh = mesh.create_unit_square(MPI.COMM_WORLD, 10, 10)
V = fem.functionspace(msh, ("Lagrange", 1))

u = ufl.TrialFunction(V)
v = ufl.TestFunction(V)
x = ufl.SpatialCoordinate(msh)

k = fem.Constant(msh, PETSc.ScalarType(1.0))
f = 10.0 * ufl.sin(ufl.pi * x[0]) * ufl.sin(ufl.pi * x[1])
```

```python

a = k * ufl.dot(ufl.grad(u), ufl.grad(v)) * ufl.dx
L = f * v * ufl.dx

# Dirichlet boundary u=0 on full boundary
fdim = msh.topology.dim - 1
boundary_facets = mesh.locate_entities_boundary(
    msh,
    fdim,
    lambda x: np.isclose(x[0], 0.0)
    | np.isclose(x[0], 1.0)
    | np.isclose(x[1], 0.0)
    | np.isclose(x[1], 1.0),
)
dofs = fem.locate_dofs_topological(V, fdim, boundary_facets)
bc = fem.dirichletbc(PETSc.ScalarType(0.0), dofs, V)

linear_problem_kwargs = {"petsc_options": {"ksp_type": "preonly", "pc_type": "lu"}}
if "petsc_options_prefix" in inspect.signature(LinearProblem).parameters:
    linear_problem_kwargs["petsc_options_prefix"] = "poisson02_"

problem = LinearProblem(a, L, bcs=[bc], **linear_problem_kwargs)
uh = problem.solve()
uh.name = "temperature"
# show some terminal output
if MPI.COMM_WORLD.rank == 0:
    print("Assembled linear system:")
    print(f"  Matrix size: {problem.A.getSize()}")

if MPI.COMM_WORLD.size == 1:
    import matplotlib.pyplot as plt

    print("  Spy of matrix (nonzeros in black):")
    row_ptr, col_idx, _ = problem.A.getValuesCSR()
    row_idx = np.repeat(np.arange(len(row_ptr) - 1), np.diff(row_ptr))
    nrows, ncols = problem.A.getSize()

    fig, ax = plt.subplots()
    ax.plot(col_idx, row_idx, "k.", markersize=0.5)
    ax.set_xlim(-0.5, ncols - 0.5)
    ax.set_ylim(nrows - 0.5, -0.5)
    ax.set_xlabel("column")
    ax.set_ylabel("row")
    ax.set_title("Sparsity pattern of the stiffness matrix")
    plt.show()
elif MPI.COMM_WORLD.rank == 0:
    print("  Spy skipped because the PETSc matrix is distributed across MPI ranks.")
```

```
Assembled linear system:
  Matrix size: (121, 121)
  Spy of matrix (nonzeros in black):
```



3.4 Simulation Output Plot

```
import matplotlib.pyplot as plt
import matplotlib.tri as mtri

tdim = msh.topology.dim
msh.topology.create_connectivity(tdim, 0)
cells = msh.topology.connectivity(tdim, 0).array.reshape(-1, 3)

nverts = msh.topology.index_map(0).size_local + msh.topology.index_map(0).num_ghosts
coords = msh.geometry.x[:nverts, :2]
vertex_ids = np.arange(nverts, dtype=np.int32)
dofs = fem.locate_dofs_topological(V, 0, vertex_ids)
u_vertex = uh.x.array[dofs].real

tri = mtri.Triangulation(coords[:, 0], coords[:, 1], triangles=cells)
fig, ax = plt.subplots(figsize=(6, 4))
pcm = ax.tripcolor(tri, u_vertex, shading="gouraud", cmap="inferno")
ax.triplot(tri, lw=0.15, color="white", alpha=0.3)
ax.set_aspect("equal")
ax.set_xlabel("x")
ax.set_ylabel("y")
ax.set_title("Temperature field $u_h$")
fig.colorbar(pcm, ax=ax, label="temperature")
plt.tight_layout()
plt.show()
```

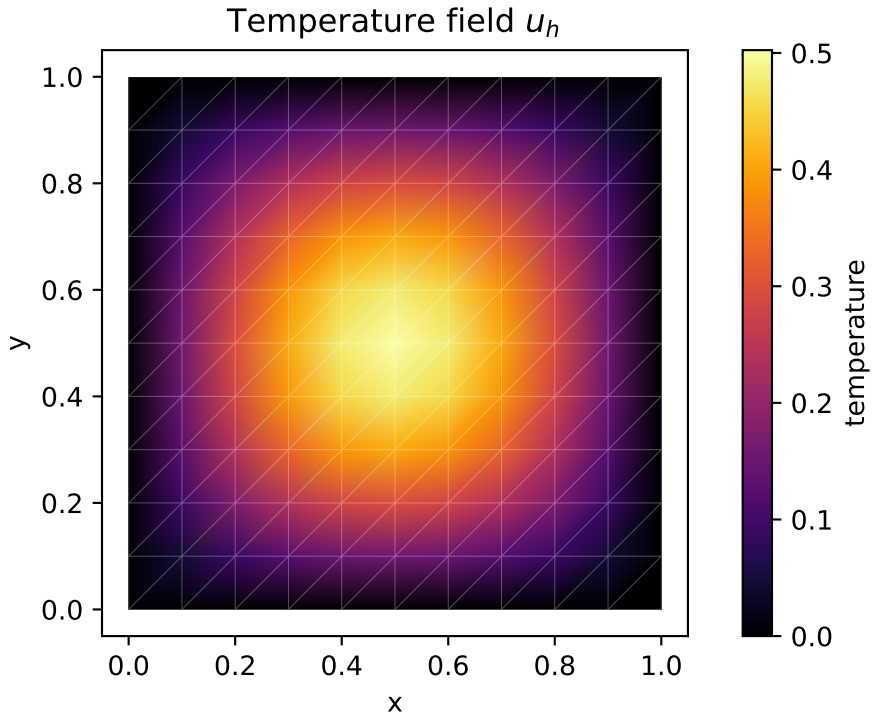


Figure 14: Lecture 02: FEM solution on the unit square

3.5 Manufactured Solution and Convergence Check

To verify an FEM implementation, we often use a *manufactured solution*: choose a smooth exact solution u_{ex}, insert it into the PDE, and derive the matching right-hand side f.

For the Poisson problem on $\Omega = (0,1)^2$, take

$$u_{\text{ex}}(x,y) = \sin(\pi x)\sin(\pi y), \qquad -\Delta u_{\text{ex}} = 2\pi^2 \sin(\pi x)\sin(\pi y),$$

with homogeneous Dirichlet boundary conditions. Since $u_{\text{ex}} = 0$ on $\partial\Omega$, it fits the same setup as before. For smooth solutions, we expect the L^2 error to behave like $O(h^{p+1})$ for Lagrange elements of degree p.

```
def solve_manufactured_problem(n, degree):
    msh = mesh.create_unit_square(MPI.COMM_WORLD, n, n)
    V = fem.functionspace(msh, ("Lagrange", degree))

    u = ufl.TrialFunction(V)
    v = ufl.TestFunction(V)
    x = ufl.SpatialCoordinate(msh)

    u_exact = ufl.sin(ufl.pi * x[0]) * ufl.sin(ufl.pi * x[1])
    f = 2.0 * ufl.pi**2 * u_exact

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

```
    fdim = msh.topology.dim - 1
    boundary_facets = mesh.locate_entities_boundary(
        msh,
        fdim,
        lambda x: np.isclose(x[0], 0.0)
        | np.isclose(x[0], 1.0)
        | np.isclose(x[1], 0.0)
        | np.isclose(x[1], 1.0),
    )
    dofs = fem.locate_dofs_topological(V, fdim, boundary_facets)
    bc = fem.dirichletbc(PETSc.ScalarType(0.0), dofs, V)

    linear_problem_kwargs = {
        "petsc_options": {"ksp_type": "preonly", "pc_type": "lu"}
    }
    if "petsc_options_prefix" in inspect.signature(LinearProblem).parameters:
        linear_problem_kwargs["petsc_options_prefix"] = f"mms_p{degree}_{n}_"

    problem = LinearProblem(a, L, bcs=[bc], **linear_problem_kwargs)
    uh = problem.solve()

    error_sq_local = fem.assemble_scalar(fem.form((uh - u_exact) ** 2 * ufl.dx))
    error_sq = msh.comm.allreduce(error_sq_local, op=MPI.SUM)
    return 1.0 / n, np.sqrt(error_sq.real)


n_values = [4, 8, 16, 32]
convergence_results = {}

for degree in (1, 2):
    hs = []
    errors = []
    for n in n_values:
        h, error_L2 = solve_manufactured_problem(n, degree)
        hs.append(h)
        errors.append(error_L2)

    hs = np.array(hs)
    errors = np.array(errors)
    orders = np.log(errors[:-1] / errors[1:]) / np.log(hs[:-1] / hs[1:])
    fitted_order = np.polyfit(np.log(hs), np.log(errors), 1)[0]

    convergence_results[degree] = {
        "h": hs,
        "error_L2": errors,
        "orders": orders,
        "fitted_order": fitted_order,
    }

if MPI.COMM_WORLD.rank == 0:
    for degree, data in convergence_results.items():
```

```
        print(f"P{degree} elements")
        print("  h         L2 error      observed order")
        for i, (h, err) in enumerate(zip(data["h"], data["error_L2"])):
            order_text = "---" if i == 0 else f"{data['orders'][i - 1]:.3f}"
            print(f"  {h:0.5f}   {err:0.6e}   {order_text}")
```

```
P1 elements
  h         L2 error      observed order
  0.25000   7.907545e-02   ---
  0.12500   2.113277e-02   1.904
  0.06250   5.377435e-03   1.974
  0.03125   1.350436e-03   1.993
P2 elements
  h         L2 error      observed order
  0.25000   4.327631e-03   ---
  0.12500   5.480619e-04   2.981
  0.06250   6.873916e-05   2.995
  0.03125   8.600535e-06   2.999
```

```
if MPI.COMM_WORLD.rank == 0:
    fig, ax = plt.subplots(figsize=(6, 4))

    for degree in (1, 2):
        data = convergence_results[degree]
        line, = ax.loglog(
            data["h"],
            data["error_L2"],
            "o-",
            linewidth=2,
            label=f"P{degree}: observed order {data['fitted_order']:.2f}",
        )
        ref = data["error_L2"][-1] * (data["h"] / data["h"][-1]) ** (degree + 1)
        ax.loglog(
            data["h"],
            ref,
            "--",
            color=line.get_color(),
            alpha=0.6,
        )

    ax.set_xlabel("mesh size h")
    ax.set_ylabel(r"$L^2$ error")
    ax.set_title("Convergence check with manufactured solution")
    ax.grid(True, which="both", linestyle=":")
    ax.legend()
    plt.tight_layout()
    plt.show()
```

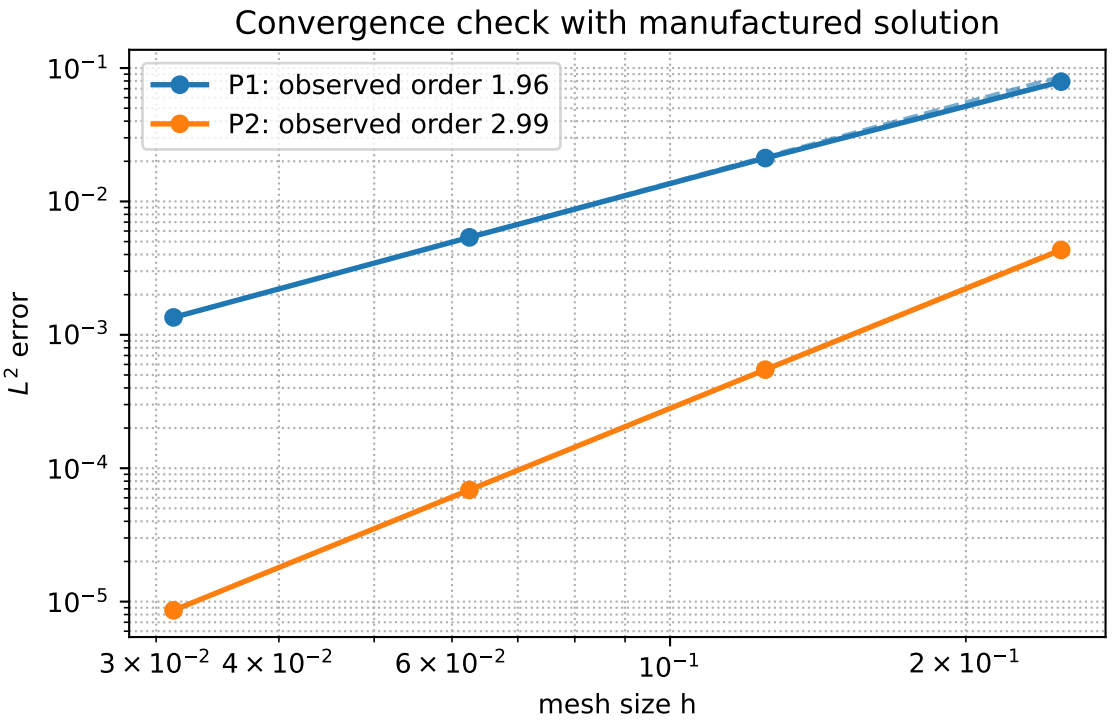


Figure 15: Manufactured-solution error in the L^2 norm for P1 and P2 elements

4 Summary

- FEM starts from a weak form and a function space setting.
- Geometry enters naturally via unstructured meshes.
- Assembly yields sparse systems suitable for modern solvers.

5 Exercises

1. Derive the weak form for a 2d reaction-diffusion equation with zero BCs and implement it in FEniCSx.
2. Extend the Poisson problem to 3D and implement it in FEniCSx. What changes in the code?
3. Derive the weak form for the equations of linear elasticity, given by

$$-\nabla \cdot \sigma = f \quad \text{in } \Omega,$$

   where σ is the stress tensor related to the displacement field u via Hooke's law $\sigma = \lambda(\nabla \cdot u)I + 2\mu\varepsilon(u)$, with $\varepsilon(u) = \frac{1}{2}(\nabla u + \nabla u^T)$ being the strain tensor, and λ and μ are the Lamé parameters. Assume appropriate boundary conditions (e.g., Dirichlet on part of the boundary and Neumann on the rest).
4. Formulate the Poisson equation as *mixed problem* by introducing an auxiliary variable $q = -k\nabla u$ (the flux), and derive the corresponding weak form. What function spaces would you choose for u and q?
5. Implement the Poisson equation with Robin boundary conditions in FEniCSx.

6 Questions

1. What are the advantages of the finite element method compared to finite difference methods, especially for complex geometries?
2. How does the choice of finite element (e.g., P1 vs P2) affect the accuracy and computational cost of the solution?
3. What are some common challenges in implementing FEM, and how does a framework like FEniCS help to address them?

7 References

- Solving the Poisson equation by Jørgen S. Dokken