# DUNE PDELab Tutorial 00

## An Introduction to the Finite Element Method

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# Motivation

- Start with an introduction to the finite element method (FEM) for solving Poisson's equation with piecewise linear "$P_1$" finite elements
- "Hello World!" for any numerical partial differential equation (PDE) solver framework!
- Gives necessary background for `dune-grid` module
- Implement the method in PDELab (Wednesday)

# Challenges for PDE Software

- **Many different PDE applications**
  - Multi-physics
  - Multi-scale
  - Inverse modeling: parameter estimation, optimal control
  - Uncertainty quantification
- **Many different numerical solution methods**
  - No single method to solve all equations!
  - Different mesh types, mesh generation, mesh refinement
  - Higher-order approximations (polynomial degree)
  - Error control and adaptive mesh/degree refinement
  - Iterative solution of (non-)linear algebraic equations
- **High-performance Computing**
  - Single core performance: Often bandwidth limited
  - Parallelization through domain decomposition
  - Robustness w.r.t. to mesh size, model parameters, processors
  - Dynamic load balancing

$\Rightarrow$ **One software to do it all!**

# Flexibility Requires Abstraction!

- DUNE/PDELab is based on an abstract formulation of the numerical scheme based on **residual forms**
- In order to implement a scheme it requires to put it to that form!
- Although you might be familiar with the FEM, you might not be familiar to the notation used here
- When you have mastered the abstraction you can solve complex problems with reasonable effort
- Important feature: Orthogonality of concepts:
  - Dimension $d = 1, 2, 3, \ldots$
  - Linear and nonlinear
  - Stationary and Instationary
  - Scalar PDE and systems of PDEs
  - Uniform and adaptive mesh refinement of different types
  - Sequential and parallel

All that will be handled in the course!

# Introduction to the Finite Element Method

# Strong Formulation of the PDE Problem

We solve Poisson's equation with inhomogeneous Dirichlet boundary conditions:

$$-\Delta u = f \qquad \text{in } \Omega, \tag{1a}$$

$$u = g \qquad \text{on } \partial\Omega, \tag{1b}$$

- $\Omega \subset \mathbb{R}^d$ is a polygonal domain in $d$-dimensional space
- A function $u \in C^2(\Omega) \cap C^0(\overline{\Omega})$ solving (1a), (1b) is called *strong solution*
- Inhomogeneous Dirichlet boundary conditions could be reduced to *homogeneous* ones: we will not do this!
- Proving existence and uniqueness of solutions of strong solutions requires quite restrictive conditions on $f$ and $g$

# Weak Formulation of the PDE Problem

Suppose $u$ is a strong solution and take *any test function* $v \in C^1(\Omega) \cap C^0(\overline{\Omega})$ with $v = 0$ on $\partial\Omega$ then:

$$\int_\Omega (-\Delta u) v \, dx = \underbrace{\int_\Omega \nabla u \cdot \nabla v \, dx}_{=:a(u,v)} = \underbrace{\int_\Omega f v \, dx}_{=:l(v)} .$$

*Question*: Is there a vector space of functions $V$ with $V_g = \{v \in V : v = g \text{ on } \partial\Omega\}$ and $V_0 = \{v \in V : v = 0 \text{ on } \partial\Omega\}$ such that the problem

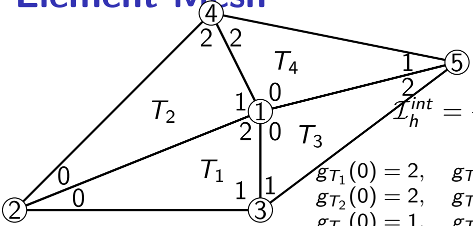
$$u \in V_g : \qquad a(u,v) = l(v) \qquad \forall v \in V_0 \tag{2}$$

has a unique solution?
*Answer*: Yes, $V = H^1(\Omega)$. This $u$ is called *weak solution*.
Advantage: Weak solutions do exist under less restrictive conditions on the data.

# The Finite Element Method

- The finite element method (FEM) is one method for the numerical solution of PDEs
- Others are the finite volume method (FVM) or the finite difference method (FDM)
- The FEM is based on the weak formulation derived above
- Its basic idea is to replace the space $V$ by a *finite-dimensional space* $V_h$!
- The construction of these finite-dimensional spaces needs some preparations . . .

# Finite Element Mesh




$\mathcal{I}_h^{int} = \{1\}, \mathcal{I}_h^{\partial\Omega} = \{2, 3, 4, 5\}$

$$\begin{aligned}
&g_{T_1}(0) = 2, \quad g_{T_1}(1) = 3, \quad g_{T_1}(2) = 1,\\
&g_{T_2}(0) = 2, \quad g_{T_2}(1) = 1, \quad g_{T_2}(2) = 4,\\
&g_{T_3}(0) = 1, \quad g_{T_3}(1) = 3, \quad g_{T_3}(2) = 5,\\
&g_{T_4}(0) = 1, \quad g_{T_4}(1) = 5, \quad g_{T_4}(2) = 4.
\end{aligned}$$

- A mesh consists of ordered sets of vertices and elements:

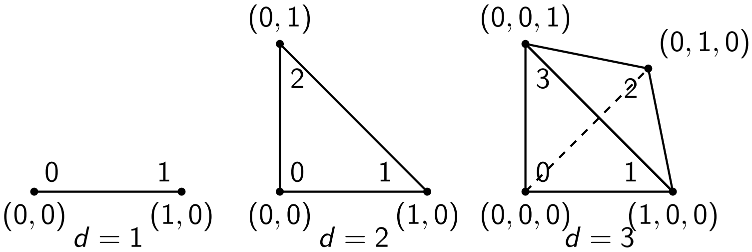
$$\mathcal{X}_h = \{x_1, \ldots, x_N\} \subset \mathbb{R}^d, \quad \mathcal{T}_h = \{T_1, \ldots, T_M\}$$

- *Simplicial element*: $T = \text{convex\_hull}(x_{T,0}, \ldots, x_{T,d})$
- *Conforming*: Intersection is subentity
- *Local to global map* : $g_T : \{0, \ldots, d\} \to \mathcal{N}$

$$\forall T \in \mathcal{T}_h, 0 \le i \le d : g_T(i) = j \Leftrightarrow x_{T,i} = x_j.$$

- *Interior and boundary vertex index sets*: $\mathcal{I}_h = \mathcal{I}_h^{int} \cup \mathcal{I}_h^{\partial\Omega}$, $\mathcal{I}_h^{int} = \{i \in \mathcal{I}_h \,:\, x_i \in \Omega\}, \mathcal{I}_h^{\partial\Omega} = \{i \in \mathcal{I}_h \,:\, x_i \in \partial\Omega\}$

# Reference Element and Element Transformation




- $\hat{T}^d$ is the reference simplex in $d$ space dimensions
- The mesh $\mathcal{T}_h$ is called *affine* if for every $T \in \mathcal{T}_h$ there is an affine linear map $\mu_T : \hat{T} \to T$,

$$\mu_T(\hat{x}) = B_T\hat{x} + a_T$$

with

$$\forall i \in \{0, \ldots, d\} : \mu_T(\hat{x}_i) = x_{T,i}$$

# Piecewise Linear Finite Element Space

- The idea of the *conforming* FEM is to solve the weak problem in *finite-dimensional* function spaces:

$$u_h \in V_{h,g} : \quad a(u_h, v) = l(v) \quad \forall v \in V_{h,0}.$$

- A particular choice is the space of *piecewise linear* functions

$$V_h(\mathcal{T}_h) = \{v \in C^0(\overline{\Omega}) \, : \, \forall T \in \mathcal{T}_h : v|_T \in \mathbb{P}_1^d\}$$

  where $\mathbb{P}_1^d = \{p : \mathbb{R}^d \to \mathbb{R} \, : \, p(x) = a^T x + b, a \in \mathbb{R}^d, b \in \mathbb{R}\}$

- One can show $\dim V_h = N = \dim \mathcal{X}_h$ and $V_h \subset H^1(\Omega)$
- *Lagrange* basis functions:

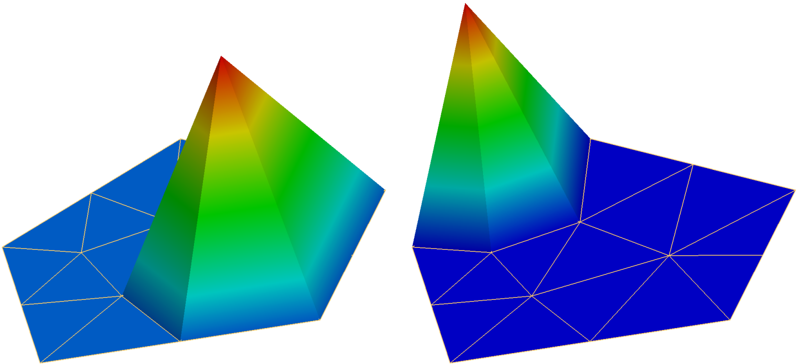
$$\Phi_h = \{\phi_1, \ldots, \phi_N\}, \quad \forall i, j \in \mathcal{I}_h \, : \, \phi_i(x_j) = \delta_{i,j}$$

- *Test and Ansatz spaces*:

$$V_{h,0} = \{v \in V_h \, : \, \forall i \in \mathcal{I}_h^{\partial\Omega} : v(x_i) = 0\},$$
$$V_{h,g} = \{v \in V_h : \forall i \in \mathcal{I}_h^{\partial\Omega} : v(x_i) = g(x_i)\} = v_{h,g} + V_{h,0}$$

# Examples of Finite Element Functions

Here in two space dimensions:



Due to their shape they are often called *hat functions*

# Finite Element Solution

Inserting a *basis representation* $u_h = \sum_{j=1}^{N} (z)_j \phi_j$ results in

$$a(u_h, v) = l(v) \quad \forall v \in V_{h,0} \quad \text{(discrete weak problem)},$$

$$\Leftrightarrow a\left(\sum_{j=1}^{N} (z)_j \phi_j, \phi_i\right) = l(\phi_i) \quad \forall i \in \mathcal{I}_h^{int} \quad \text{(insert basis, linearity)},$$

$$\Leftrightarrow \sum_{j=1}^{N} (z)_j a\left(\phi_j, \phi_i\right) = l(\phi_i) \quad \forall i \in \mathcal{I}_h^{int} \quad \text{(linearity)}.$$

Together with the condition $u_h \in V_{h,g}$ expressed as

$$u_h(x_i) = z_i = g(x_i) \quad \forall i \in \mathcal{I}_h^{\partial\Omega}$$

this forms a system of linear equations

$$Ax = b$$

where

$$(A)_{i,j} = \begin{cases} a(\phi_j, \phi_i) & i \in \mathcal{I}_h^{int} \\ \delta_{i,j} & i \in \mathcal{I}_h^{\partial\Omega} \end{cases}, \quad (b)_i = \begin{cases} l(\phi_i) & i \in \mathcal{I}_h^{int} \\ g(x_i) & i \in \mathcal{I}_h^{\partial\Omega} \end{cases}.$$

# Solution of Linear Systems

- *Exact* solvers based on Gaussian elimination
- This may become inefficent for *sparse* linear systems
- *Iterative* methods (hopefully) produce a convergent sequence

$$\lim_{k\to\infty} z^k = z$$

- A very simple example is *Richardson's* iteration:

$$z^{k+1} = z^k + \omega(b - Az^k)$$

  requiring only *matrix-vector products*
- Another well known class of iterative solvers are Krylov methods requiring also only matrix-vector products

# Three Steps to Solve the FE Problem

1. Assembling the matrix $A$. This mainly involves the computation of the matrix elements $a(\phi_j, \phi_i)$ and storing them in an appropriate data structure.
2. Assembling the right hand side vector $b$. This mainly involves evaluations of the right hand side functional $l(\phi_i)$.
3. *Alternatively:* Perform a matrix free operator evaluation $y = Az$. This involves evaluations of $a(u_h, \phi_i)$ for all test functions $\phi_i$ and a given function $u_h$ due to:

$$\begin{aligned}(Az)_i = \sum_{j=1}^{N} (A)_{i,j}(z)_j &= \sum_{j=1}^{N} a(\phi_j, \phi_i)(z)_j \\ &= a\left(\sum_{j=1}^{N} (z)_j \phi_j, \phi_i\right) = a(u_h, \phi_i)\end{aligned}$$

We now discuss *how* these steps may be implemented

# Four Important Tools

1. Transformation formula for integrals. For $T \in \mathcal{T}_h$:

$$\int_T y(x)\,dx = \int_{\hat{T}} y(\mu_T(\hat{x}))|\det B_T|\,dx.$$

2. Midpoint rule on the reference element:

$$\int_{\hat{T}} q(\hat{x})\,dx \approx q(\hat{S}_d)w_d$$

(More accurate formulas are used later)

3. Basis functions via shape function transformation:

$$\hat{\phi}_0(\hat{x}) = 1 - \sum_{i=1}^{d} (\hat{x})_i, \quad \hat{\phi}_i(\hat{x}) = (\hat{x})_i, i > 0, \quad \phi_{T,i}(\mu_T(\hat{x})) = \hat{\phi}_i(\hat{x})$$

4. Computation of gradients. For any $w(\mu_T(\hat{x})) = \hat{w}(\hat{x})$:

$$B_T^T \nabla w(\mu_T(\hat{x})) = \hat{\nabla}\hat{w}(\hat{x}) \quad \Leftrightarrow \quad \nabla w(\mu_T(\hat{x})) = B_T^{-T}\hat{\nabla}\hat{w}(\hat{x}).$$

# Assembly of Right Hand Side I

In computing $(b)_i$ only the following elements are involved:

$$C(i) = \{(T, m) \in \mathcal{T}_h \times \{0, \ldots, d\} \, : \, g_T(m) = i\}$$

Then

$$\begin{aligned}
(b)_i = l(\phi_i) &= \int_\Omega f \phi_i \, dx && \text{(definition)} \\
&= \sum_{T \in \mathcal{T}_h} \int_T f \phi_i \, dx && \text{(use mesh)} \\
&= \sum_{(T,m) \in C(i)} \int_{\hat{T}} f(\mu_T(\hat{x})) \hat{\phi}_m(\hat{x}) |\det B_T| \, dx && \text{(localize)} \\
&= \sum_{(T,m) \in C(i)} f(\mu_T(\hat{S}_d)) \hat{\phi}_m(\hat{S}_d) |\det B_T| w_d + \text{err.} && \text{(quadrature)}
\end{aligned}$$

# Assembly of Right Hand Side II

- Now we need to perform these computations *for all* $i \in \mathcal{I}_h^{int}$!
- Collect *element-local* computations:

$$(b_T)_m = f(\mu_T(\hat{S}_d))\hat{\phi}_m(\hat{S}_d)|\det B_T|w_d \quad \forall m = 0, \dots, d$$

- Define restriction matrix $R_T : \mathbb{R}^N \to \mathbb{R}^{d+1}$ with

$$(R_T x)_m = (x)_i \quad \forall\, 0 \le m \le d,\ g_T(m) = i,$$

- Then

$$b = \sum_{T \in \mathcal{T}_h} R_T^T b_T.$$

# Assembly of Global Stiffness Matrix I

In computing $(A)_{i,j}$ only the following elements are involved:

$$C(i,j) = \{(T, m, n) \in \mathcal{T}_h \times \{0, \ldots, d\} \,:\, g_T(m) = i \wedge g_T(n) = j\}$$

Then

$$\begin{aligned}
(A)_{i,j} &= a(\phi_j, \phi_i) = \int_\Omega \nabla\phi_j \cdot \nabla\phi_i \, dx && \text{(definition)}\\
&= \sum_{T \in \mathcal{T}_h} \int_T \nabla\phi_j \cdot \nabla\phi_i \, dx && \text{(use mesh)}\\
&= \sum_{(T,m,n) \in C(i,j)} \int_{\hat{T}} (B_T^{-T} \hat{\nabla}\hat{\phi}_n(\hat{x})) \cdot (B_T^{-T} \hat{\nabla}\hat{\phi}_m(\hat{x})) |\det B_T| \, d\hat{x} && \text{(localize)}\\
&= \sum_{(T,m,n) \in C(i,j)} (B_T^{-T} \hat{\nabla}\hat{\phi}_n(\hat{S}_d)) \cdot (B_T^{-T} \hat{\nabla}\hat{\phi}_m(\hat{S}_d)) |\det B_T| w_d. && \text{(quadrature}
\end{aligned}$$

# Assembly of Global Stiffness Matrix II

- Now we need to perform these computations for *all* matrix entries!
- Define the $d \times d+1$ matrix of shape function gradients

$$\hat{G} = \left[\hat{\nabla}\hat{\phi}_0(\hat{S}_d)), \ldots, \hat{\nabla}\hat{\phi}_d(\hat{S}_d))\right].$$

  and the matrix of transformed gradients

$$G = B_T^{-T}\hat{G}$$

- Define the *local stiffness matrix*

$$A_T = G^T G |\det B_T| w_d.$$

- Then

$$A = \sum_{T \in \mathcal{T}_h} R_T^T A_T R_T.$$

# Matrix-free Operator Evaluation

- Similar considerations apply for the operation $y = Az$
- Pick out the coefficients on the element $T$:

$$z_T = R_T z$$

- Perform the *element-local computation*:

$$y_T = |\det B_T| w_d G^T G z_T$$

- Accumulate the results:

$$Az = \sum_{T \in \mathcal{T}_h} R_T^T y_T.$$

# Implementation Summary

- All necessary steps in the solution procedure have the following general form:

  1: **for** $T \in \mathcal{T}_h$ **do** ▷ loop over mesh elements
  2: $\quad z_T = R_T z$ ▷ load element data
  3: $\quad q_T = \text{compute}(T, z_T)$ ▷ element local computations
  4: $\quad \text{Accumulate}(q_T)$ ▷ store result in global data structure
  5: **end for**

- PDELab provides a generic *assembler* that performs all these steps, except (3) which needs to be supplied by the implementor of a FEM
- All these concepts carry over to
  - Nonlinear problems
  - Time-dependent problems
  - Systems of PDEs
  - High-order methods
  - Other schemes such as FVM, nonconforming FEM
  - Parallel computations

# Residual Forms

- The FEM based on the weak formulation formulation may equivalently be written as

$$\text{Find } u_h \in U_h \text{ s.t.:} \quad r_h^{\text{Poisson}}(u_h, v) = 0 \quad \forall v \in V_h.$$

  where $r^{\text{Poisson}}(u_h, v) = a(u_h, v) - l(v)$ is the **residual form**
- This residual form is *affine linear* in $u_h$ and *linear* in $v$
- A *nonlinear* PDE results in a residual form $r(u, v)$ that is *nonlinear* in its first argument
- Residual forms are always linear in the second argument due to linearity of the integral
- **PDELab uses the concept of a residual form as its main abstraction!**

# Generalization

- More complicated discretization schemes:

$$
\begin{aligned}
r(u,v) = \sum_{T\in\mathcal{T}_h} \alpha_T^V(R_T u, R_T v) + \sum_{T\in\mathcal{T}_h} \lambda_T^V(R_T v) \\
+ \sum_{F\in\mathcal{F}_h^i} \alpha_F^S(R_{T_F^-} u, R_{T_F^+} u, R_{T_F^-} v, R_{T_F^+} v) \\
+ \sum_{F\in\mathcal{F}_h^{\partial\Omega}} \alpha_F^B(R_{T_F^-} u, R_{T_F^-} v) + \sum_{F\in\mathcal{F}_h^{\partial\Omega}} \lambda_F^B(R_{T_F^-} v).
\end{aligned}
$$

- Instationary problems: Find $u_h(t) \in U_h$ s.t.:

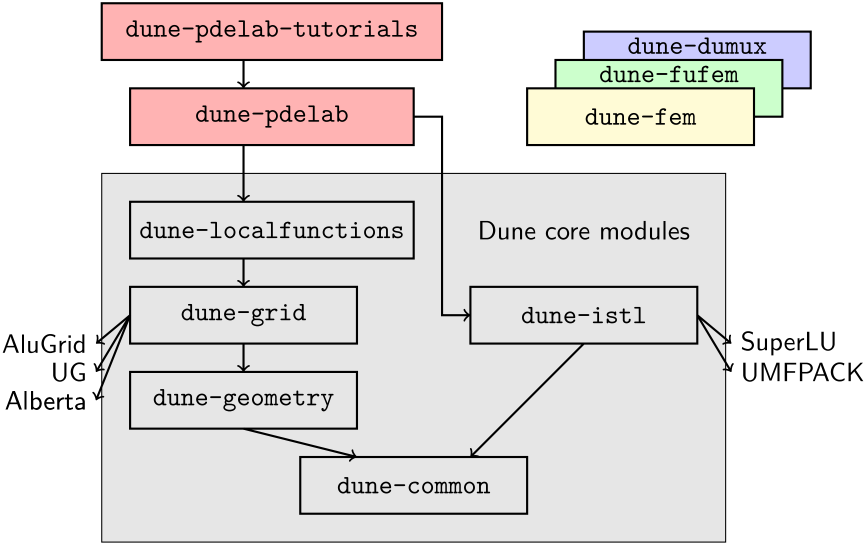
$$
d_t m_h(u_h(t), v; t) + r_h(u_h(t), v; t) = 0 \quad \forall v \in V_h
$$

- Systems of PDEs: Find $u_h \in U_h = U_h^1 \times \ldots \times U_h^s$ s.t.:

$$
r_h(u_h, v) = 0 \quad \forall v \in V_h = V_h^1 \times \ldots \times V_h^s
$$

# Implementation in DUNE/PDELab

# The Duniverse



# The PDE Problem Revisited

We solve Poisson's equation with inhomogeneous Dirichlet boundary conditions:

$$\begin{aligned} -\Delta u &= f \qquad \text{in } \Omega \\ u &= g \qquad \text{on } \partial\Omega \end{aligned}$$

The weak formulation is

$$u \in V_g : \qquad a(u, v) = l(v) \qquad \forall v \in V_0$$

with

$$a(u, v) = \int_\Omega \nabla u \cdot \nabla v \, dx \quad \text{and} \quad l(v) = \int_\Omega fv \, dx$$

and

$$\begin{aligned} &V_0 = H_0^1(\Omega) \\ &V_g = \{v \in H^1(\Omega) \, : \, v = u_g + w \wedge u_g|\Gamma_D = g \wedge w \in V_0\} \end{aligned}$$

# Generic Assembly Loop

**for** $T \in \mathcal{T}_h$ **do** ▷ loop over mesh elements
    $z_T = R_T z$ ▷ load element data
    $q_T = \text{compute}(T, z_T)$ ▷ element local computations
    Accumulate$(q_T)$ ▷ store result in global data structure
**end for**

Only the computational kernels compute$(T, z_T)$ need to be implemented by the user to implement the finite element method

# Assembly of Right Hand Side

- Now we need to perform these computations *for all* $i \in \mathcal{I}_h^{int}$!
- Collect *element-local* computations:

$$(b_T)_m = f(\mu_T(\hat{S}_d))\hat{\phi}_m(\hat{S}_d)|\det B_T|w_d \quad \forall m = 0, \dots, d$$

- Define destriction matrix $R_T : \mathbb{R}^N \to \mathbb{R}^{d+1}$ with

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- Then

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- Define the $d \times d+1$ matrix of shape function gradients

$$\hat{G} = \left[\hat{\nabla}\hat{\phi}_0(\hat{S}_d)), \ldots, \hat{\nabla}\hat{\phi}_d(\hat{S}_d))\right].$$

  and the matrix of transformed gradients

$$G = B_T^{-T}\hat{G}$$

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# Matrix-free Operator Evaluation

- Similar considerations apply for the operation $y = Az$
- Pick out the coefficients on the element $T$:

$$z_T = R_T z$$

- Perform the *element-local computation*:

$$y_T = |\det B_T| w_d G^T G z_T$$

- Accumulate the results:

$$Az = \sum_{T \in \mathcal{T}_h} R_T^T y_T.$$

# Overview DUNE/PDELab Implementation

Files involved are:

1) File `tutorial00.cc`
   - Includes C++, DUNE and PDELab header files
   - Includes all the other files
   - Contains the `main` function
   - Creates a finite element mesh and calls the `driver`
2) File `tutorial00.ini`
   - Contains parameters controlling the execution
3) File `driver.hh`
   - Function `driver` setting up and solving the finite element problem
4) File `poissonp1.hh`
   - Class `PoissonP1` realizing the necessary element-local computations

Now lets go to the code ...