Introduction to Finite Element Methods

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(original slides by Peter Bastian with modifications from Claus-Justus Heine as part of the PDELab tutorial and Geilo Summerschool 2019,

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 Python bindings of the `dune-fem` module
- Implementation of Newmark Methods for solving ODEs

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-Fem and also DUNE-PDELab are 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 (see examples with UFL)
- 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

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.

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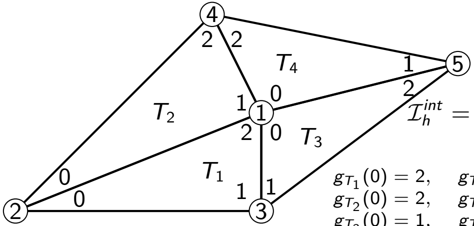
The Finite Element Method

- 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:

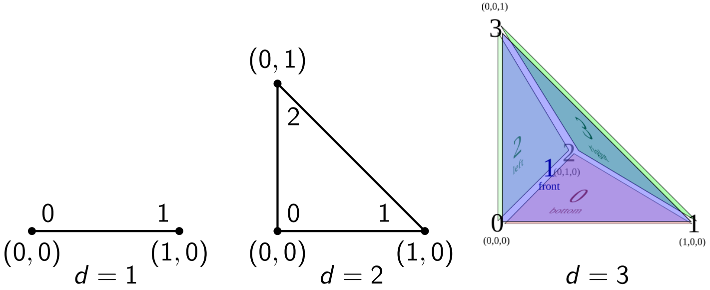
$$\mathcal{X}_h = \{x_1, \ldots, x_N\} \subset \mathbb{R}^d, \quad \mathcal{T}_h = \{T_1, \ldots, T_M\}$$

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

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

- *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 $F_T : \hat{T} \to T$,

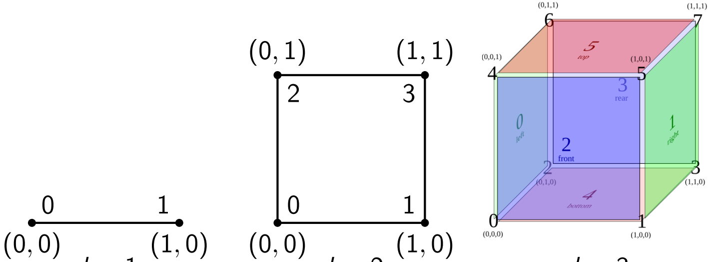
$$F_T(\hat{x}) = B_T \hat{x} + q_T$$

  with

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

Reference Element and Element Transformation

cont. Cube Mesh



$d = 1$ $d = 2$ $d = 3$

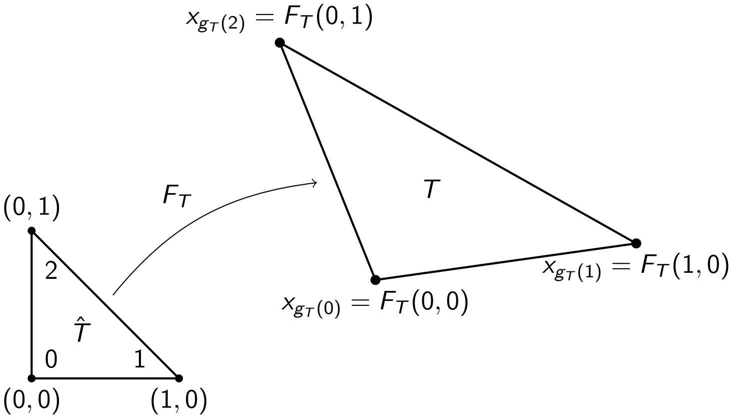
- $\hat{Q}^d$ is the reference cube in d space dimensions
- normally one uses d-linear interpolation F_Q between the vertices of $\hat{Q}^d$ and a d-"cuboid",

$$F_Q(\hat{x}_i) = x_{g_Q(i)}, \quad i = 0, ..., (2^d - 1)$$

- the mapping between $\hat{Q}^d$ and a general d-"cuboid" Q cannot be linear in general

Reference Element and Element Transformation

cont.



- Reference mapping $F_T : \hat{T} \to T : \hat{x} \mapsto F_T(\hat{x}) = B_T\hat{x} + x_{g_T(0)}$.
- Integration element $|\det(B_T)| = |\det(\hat{\nabla} F_T)|$.

Piecewise Linear Finite Element Space

- The idea of the *conforming* FEM is to solve the weak problem in *finite-dimensional* function spaces $V_h \subset V$:

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

- 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:

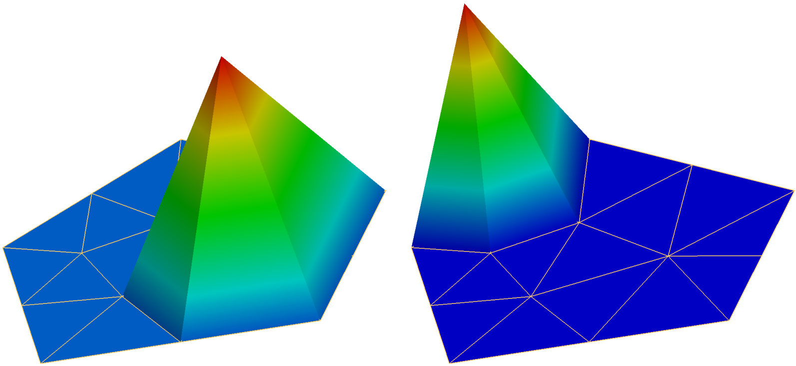
$$\Phi_h = \{\phi_1, \ldots, \phi_N\}, \quad \forall i,j \in \mathcal{I}_h \,:\, \phi_i(x_j) = \delta_{i,j}$$

- *Test and Ansatz (Trial) 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*

Construction of Finite Element Basis Functions

- Define "shape functions" $\hat{\phi}_i$ on the reference element
- Construct global basis functions ϕ_k for $k = g_T(i)$ by a "pull-back"

$$\phi_k|_T(x) := \hat{\phi}_i(F_T^{-1}(x)) \;\Leftrightarrow\; \phi_k|_T(F_T(\hat{x})) = \hat{\phi}_i(\hat{x}).$$

Example for Lagrange functions on simplices: use e.g. "barycentric coordinates"

$$\lambda_0(\hat{x}) = 1 - \sum_{i=1}^{d} \hat{x}_i, \quad \lambda_i(\hat{x}) = \hat{x}_i \;(i > 0), \quad F_T(\hat{x}) = \sum_{i=0}^{d} \lambda_i(\hat{x})\, x_{g_T(i)}.$$

- Linear: $\hat{\phi}_i = \lambda_i$, $i = 0, \ldots, d$
- Quadratic: ...

Finite Element Solution

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

$$
\begin{aligned}
a(u_h, v) &= l(v) \quad \forall v \in V_{h,0} \quad &&\text{(discrete weak problem)}, \\
\Leftrightarrow a\left(\sum_{j=1}^{N} (z)_j \phi_j, \phi_i\right) &= l(\phi_i) \quad \forall i \in \mathcal{I}_h^{int} \quad &&\text{(insert basis, linearity)}, \\
\Leftrightarrow \sum_{j=1}^{N} (z)_j a\left(\phi_j, \phi_i\right) &= l(\phi_i) \quad \forall i \in \mathcal{I}_h^{int} \quad &&\text{(linearity)}.
\end{aligned}
$$

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 ϕ_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 $T \in \mathcal{T}_h$:

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

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:

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

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

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

Assembly of Right Hand Side I

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

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

Then

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

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:

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

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

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

- 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

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

Implementation Summary

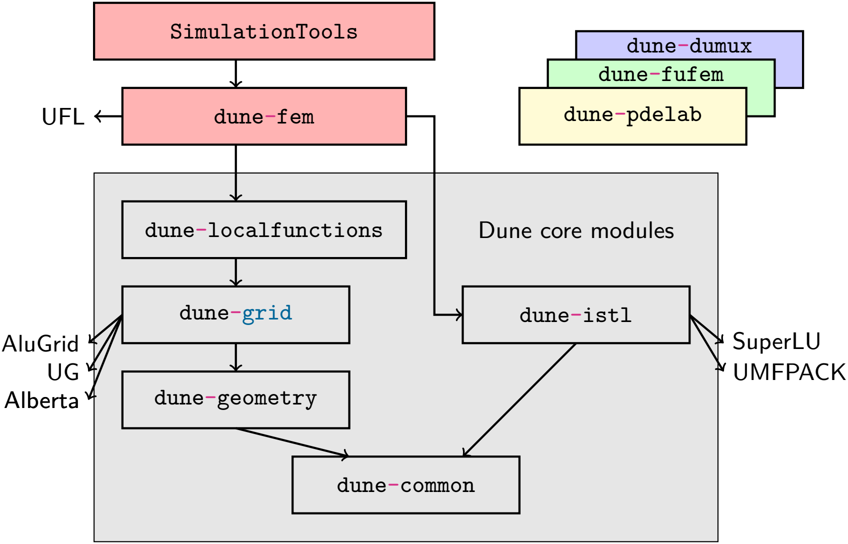
- All necessary steps in the solution procedure have the following general form:

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

- DUNE-Fem provides a generic *assembler (galerkin scheme)* that performs all these steps, except (3) which needs to be supplied by the implementor using UFL forms
- 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

Implementation in DUNE-Fem

The Duniverse

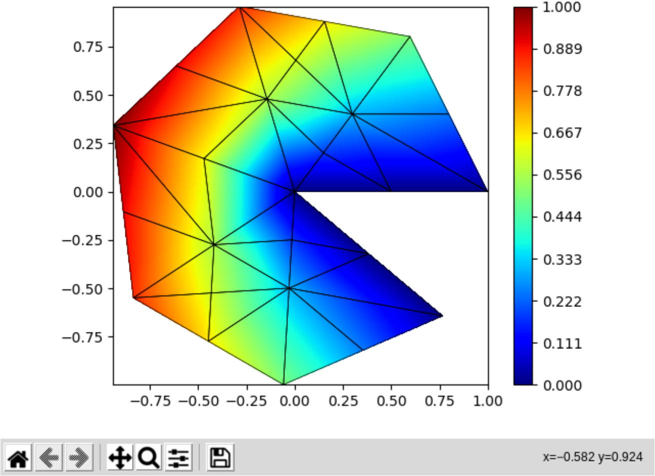


Laplace example

laplace.py

```
vertices = numpy.zeros((8, 2))
vertices[0] = [0, 0]
for i in range(0, 7):
    vertices[i+1] = [math.cos(cornerAngle/6*math.pi/180*i),
                     math.sin(cornerAngle/6*math.pi/180*i)]
triangles = numpy.array([[2,1,0], [0,3,2], [4,3,0],
                         [0,5,4], [6,5,0], [0,7,6]])

domain = {"vertices": vertices, "simplices": triangles}
gridView = adaptiveGridView( leafGridView(domain) )

gridView.hierarchicalGrid.globalRefine(2)
space = solutionSpace(gridView, order=1, storage="istl")

u = TrialFunction(space)
v = TestFunction(space)
x = SpatialCoordinate(space.cell())

# exact solution for this angle
Phi = cornerAngle / 180 * pi
phi = atan_2(x[1], x[0]) + conditional(x[1] < 0, 2*pi, 0)
# u = g on the boundary
exact = dot(x, x)**(pi/2/Phi) * sin(pi/Phi * phi)
a = dot(grad(u), grad(v)) * dx

# set up the scheme
from dune.fem.scheme import galerkin as solutionScheme
laplace = solutionScheme([a==0, DirichletBC(space, exact, 1)], solver="cg",
            parameters={"newton.linear.preconditioning.method":"ilu"})
uh = space.interpolate([0], name="solution")

laplace.solve(target=uh)

uh.plot()
```

Result



0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−0.75 −0.50 −0.25 0.00 0.25 0.50 0.75 1.00
1.000
0.889
0.778
0.667
0.556
0.444
0.333
0.222
0.111
0.000
x=−0.582 y=0.924

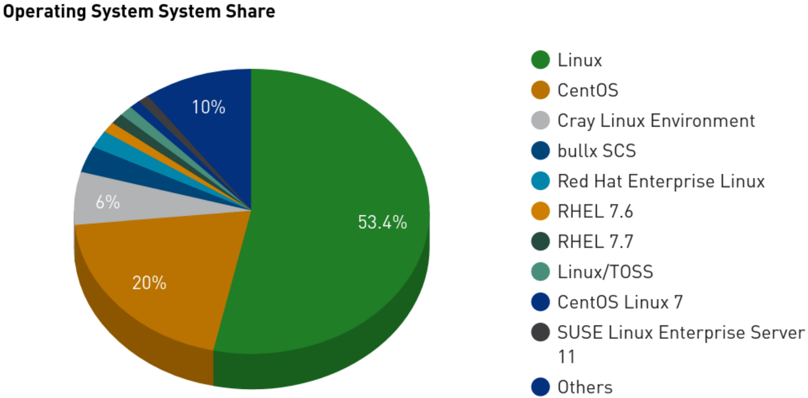
Software installation

Poll

What is the percentage of Linux systems on the worlds top 500 super computers?

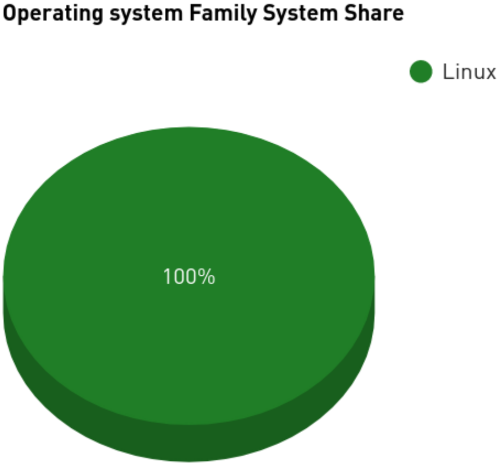
- $0 - 49\%$ Write A in chat
- $50 - 74\%$ Write B in chat
- $75 - 99\%$ Write C in chat
- 100% Write D in chat

Top 500 Super Computers in the World



https://top500.org/statistics/list/

Top 500 Super Computers in the World



https://top500.org/statistics/list/

Further Reading

Tutorial dune-fem
https://dune-project.org/sphinx/content/sphinx/dune-fem/
Accessed February 10, 2023.