Three Week Presentation

Building blocks for Finite Element computations in IPPL

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1. Problem
2. FEM Introduction
3. My Task and Timeline
4. Implementation
   - Software Architecture
   - Finite Element Space class: Mesh mapping and Basis Functions
   - Element Classes and Transformations
5. Future

Problem

- Usecase for FEM in IPPL
  - Goal: Solving Maxwell equations
  - FDTD is 2nd order, FEM can be higher accuracy
- Arguments against external libraries
  - Avoiding data copies
  - Less coupling to external libraries, more modularity
  - More control: exascale, performant, portable FEM in IPPL

Finite Element Method

- Formulate the PDE in variational formulation:
  Example: Poisson Equation

$$\begin{cases} -\Delta \boldsymbol{u} = \boldsymbol{f} & \text{in } \Omega \\ \boldsymbol{u} = \boldsymbol{0} & \text{on } \partial\Omega \end{cases} \quad \Rightarrow \quad \int_\Omega \nabla \boldsymbol{u} \cdot \nabla \boldsymbol{v} = \int_\Omega \boldsymbol{f} \cdot \boldsymbol{v} \quad \forall \boldsymbol{v} \in V$$

- Mesh the domain with Elements: $\Omega = \bigcup_{e=1}^{N_E} K_e$
- Each element has a corresponding local system of equations: $\mathbf{A}_K \boldsymbol{x} = \boldsymbol{b}_K$
- Assemble the global system of equations

$$\mathbf{A}\boldsymbol{x} = \boldsymbol{b}$$

This system of equations can be solved matrix-free!

Conjugate Gradient (CG) Method

- Matrix-free, avoids building the global FEM matrix
- Iterative algorithm, terminates when remainder is sufficiently small
- Relies on the "action" of the matrix on a vector.

CG evaluates $\mathbf{A}\boldsymbol{x}$, with a given $\boldsymbol{x}$, every iteration.
Requires $\boldsymbol{b}$ at the beginning of the algorithm.

Building blocks

- Evaluate basis functions (and their gradient) on elements
- Transformation from local to global coordinate system for element
- Numerical integration rule using polynomial interpolation on element
- Functions to interface FEM with CG.

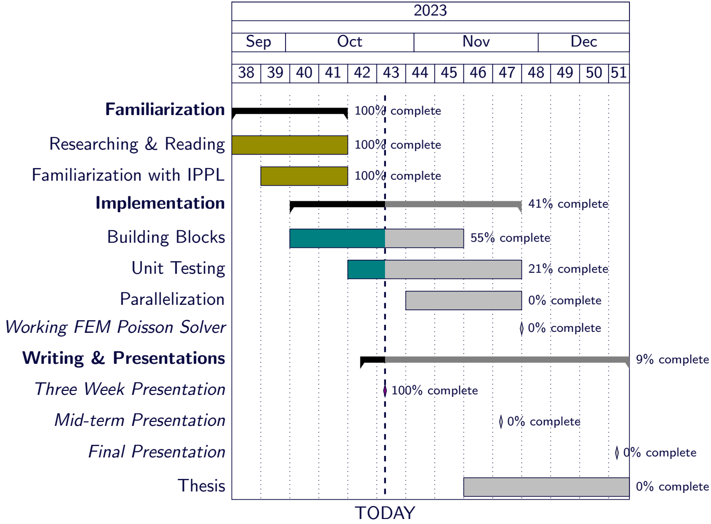
My Task

Task: Implementation of the building blocks and corresponding unit tests in IPPL.

Building blocks:

1. Reference element base class and child element classes with local to global transformations for
   - Edge (1D)
   - Quadrilateral (2D)
   - Hexahedral (3D)
2. Finite element space base class
   - Mesh (and vertices) to elements mapping
   - Child classes with corresponding basis functions for the FEM spaces:
     - Lagrange
     - Nédélec
     - Raviart-Thomas
3. Quadrature rule base class and Gauss-Jacobi quadrature rule

Timeline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100% complete
Researching & Reading
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Familiarization with IPPL
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Implementation
41% complete
Building Blocks
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Unit Testing
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Parallelization
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Working FEM Poisson Solver
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Writing & Presentations
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Final Presentation
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Thesis
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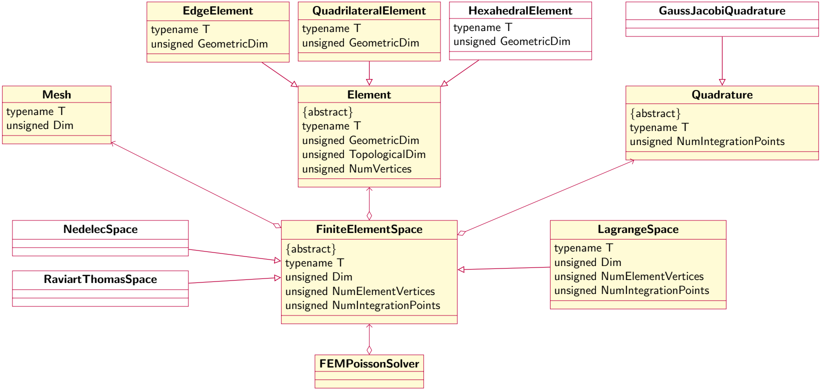
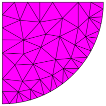
TODAY

Software Architecture



Mesh types

- Unstructured Mesh



- Structured Mesh

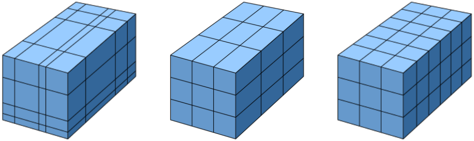


Figure: Rectilinear mesh, Regular mesh, Cartesian mesh[1]

⇒ IPPL Only has structured meshes

[1] Source: Wikimedia Commons. Drawn by SIffea, vectorized by Mysid.

Mesh: Element and Vertex mapping

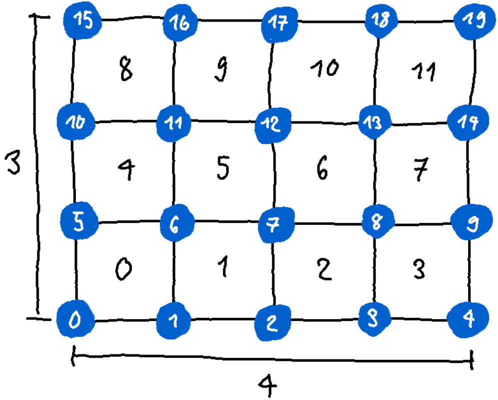


Figure: Example 4×3 2D regular mesh

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Basis functions

$$b_h^j(x_i) = \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

Lagrange 1st order shape functions:

- 1D: $x \in [0, 1]$

$$b_h^1 = 1 - x$$
$$b_h^2 = x$$

- 2D: $(x, y) \in [0, 1]^2$

$$b_h^1 = (1 - x)(1 - y)$$
$$b_h^2 = x(1 - y)$$
$$b_h^3 = (1 - x)y$$
$$b_h^4 = xy$$

Finite Element Spaces: Lagrange (1st order) 1D

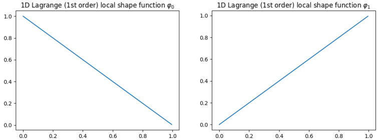


Figure: Local Shape functions for 1D 1st order Lagrange

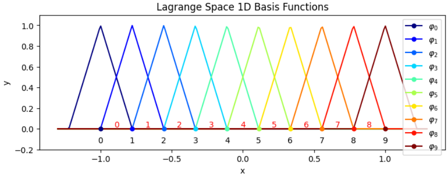


Figure: Shape functions of 1D uniform mesh with ten DoFs. (1D 1st order Lagrange)

Finite Element Spaces: Lagrange (1st order) 2D

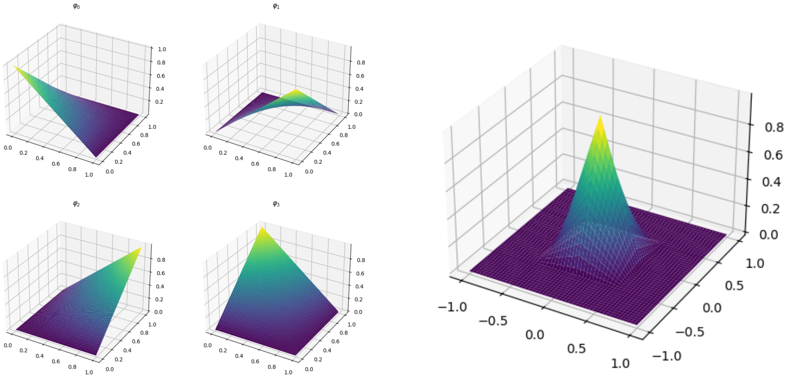


Figure: Left: local shape functions, Right: Basis of Node 12 on 5x5 mesh (2D 1st order Lagrange)

FiniteElementSpace Class

Elements: Local mapping

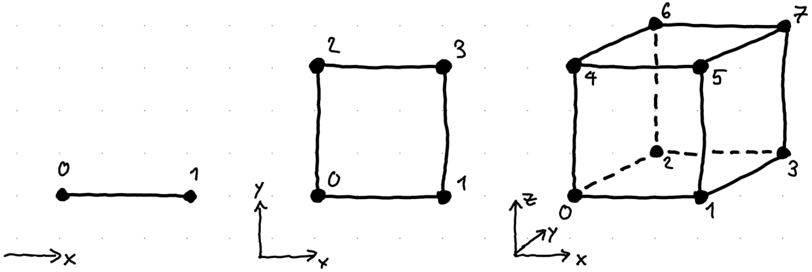
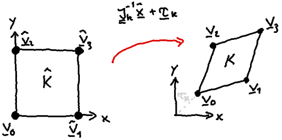


Figure: Local vertex mapping for EdgeElement, QuadrilateralElement, HexahedralElement (from left to right)

Element Transformations

- Transformation to and from local and global coordinates using affine transfomations



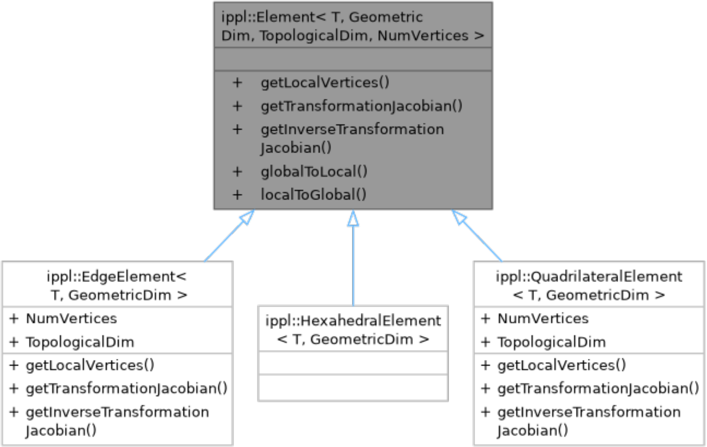
- Local to Global: $\boldsymbol{x} = \mathbf{J}_K^{-1}\hat{\boldsymbol{x}} + \boldsymbol{\tau}_K$,with $\boldsymbol{\tau}_K = \boldsymbol{v}_0$

$$\mathbf{J}_K^{-1} := \begin{bmatrix} \boldsymbol{v}_x^1 - \boldsymbol{v}_x^0 & \boldsymbol{v}_x^2 - \boldsymbol{v}_x^0 \\ \boldsymbol{v}_y^1 - \boldsymbol{v}_y^0 & \boldsymbol{v}_y^2 - \boldsymbol{v}_y^0 \end{bmatrix} \quad \text{(General)}$$

$$\mathbf{J}_K^{-1} := \begin{bmatrix} \boldsymbol{v}_x^1 - \boldsymbol{v}_x^0 & 0 \\ 0 & \boldsymbol{v}_y^2 - \boldsymbol{v}_y^0 \end{bmatrix} \quad \text{(Grid, only scaling)}$$

- Global to Local: $\hat{\boldsymbol{x}} = \mathbf{J}_K(\boldsymbol{x} - \boldsymbol{\tau}_K)$

Element Classes



Plan for the (near) future

- Currently working on: Element transformations.
- Next steps:
  1. Implement `evaluateAx`, `evaluateLoadVector`
  2. Implement Gauss-Jacobi Quadrature
  3. Going from 1D and 2D to 3D
  4. Thread- and Process-level Parallelization

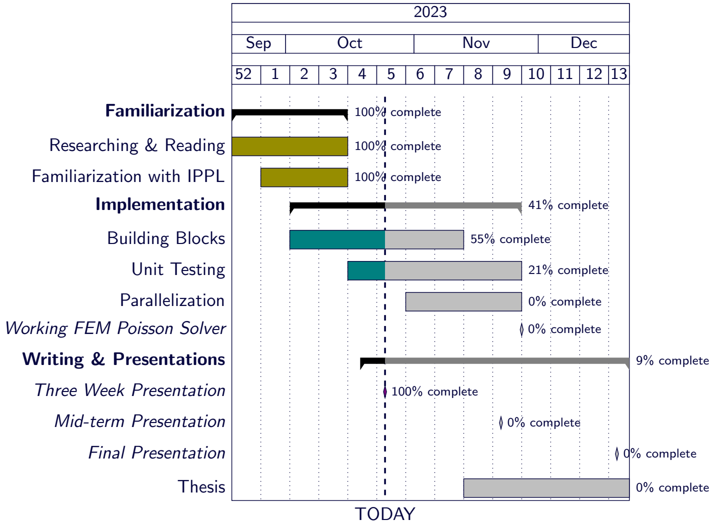
Add unit tests continually to test completed implementations.

References

[Hiptmair NumCSE] R. Hiptmair. Numerical Methods for Computational Science and Engineering. 2019. URL: https://www.sam.math.ethz.ch/ gr-sam/NCSE20/NumCSE_Lecture_Document.pdf

[Hiptmair NumPDE] R. Hiptmair. Numerical Methods for (Partial) Differential Equations. 2022. URL: https://www.sam.math.ethz.ch/ grsam/NUMPDEFL/NUMPDE.pdf

Timeline



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Appendix A: Quadrature

m-point quadrature rule on $[a, b]$, $m \in \mathbb{N}$

$$\int_a^b f(t)\, \mathrm{d}t \approx \sum_{j=1}^{m} w_j\, f(p_j) \tag{1}$$

where $w_j \in \mathbb{R}$ are the quadrature weights and $\boldsymbol{p}_j$ quadrature nodes $\in [a, b]$.

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Appendix B: Pseudo-code

evaluateAx($\boldsymbol{x}$)

$z \leftarrow 0$

for $\underline{i \leftarrow 0}$ **to** $\underline{N_{\text{DoFs}};\ i = i + 1}$ **do**

  $\mathbf{J}^{-1}, det\mathbf{J} \leftarrow$ `getInverseTransformationJacobian`(element)

  `evaluatePDE`$(i, j, \boldsymbol{q}_k) \ \leftarrow \ \mathbf{J}^{-1}\nabla\boldsymbol{\varphi}_i(\boldsymbol{q}_k) \cdot \mathbf{J}^{-1}\nabla\boldsymbol{\varphi}_j(\boldsymbol{q}_k)$

  for $\underline{j \leftarrow 0}$ **to** $\underline{N_{\text{DoFs}};\ j = j + 1}$ **do**

    $\mathbf{A}_{ij}^{K} \leftarrow \sum_{k=0}^{N_I} w_k \cdot$ `evaluatePDE`$(i, j, \boldsymbol{q}_k)$

    $z \leftarrow z + A_{ij}^{K}\boldsymbol{x}_j$

  end

end

Algorithm 1: `evaluateAx` (Poisson equation)

Appendix C: Example: Poisson Equation - Strong to weak formulation

- Poisson equation in strong form, with Dirichlet boundary conditions and given source term $\boldsymbol{f}$.

$$\begin{aligned} -\Delta \boldsymbol{u} &= \boldsymbol{f} \quad \text{in } \Omega \\ \boldsymbol{u} &= \mathbf{0} \quad \text{on } \partial\Omega \end{aligned} \tag{2}$$

- Integral equation

$$-\int_\Omega \Delta \boldsymbol{u} \cdot \boldsymbol{v} = \int_\Omega \boldsymbol{f} \cdot \boldsymbol{v} \quad \forall \boldsymbol{v} \in V$$

- Weak form of the Poisson equation

$$\int_\Omega \nabla \boldsymbol{u} \cdot \nabla \boldsymbol{v} = \int_\Omega \boldsymbol{f} \cdot \boldsymbol{v} \quad \forall \boldsymbol{v} \in V \tag{3}$$

Appendix C: Example: Poisson Equation - Discretization

- Restrict spaces: $v, u \in V_h \subset V$ (Galerkin finite element method)
- Space discretization (Meshing) $\quad \Omega = \bigcup_{e=1}^{N_E} K_e$

$$\sum_{e=1}^{N_E} \int_{K_e} \nabla \boldsymbol{u} \cdot \nabla \boldsymbol{v} = \sum_{e=1}^{N_E} \int_{K_e} \boldsymbol{f} \cdot \boldsymbol{v} \quad \forall \boldsymbol{v} \in V_h$$

- Write functions in terms of the basis functions

$$\boldsymbol{u} = \sum_i u_i \boldsymbol{\varphi}_i, \quad \boldsymbol{v} = \sum_j v_j \boldsymbol{\varphi}_j$$

$$\sum_i u_i \sum_{e=1}^{N_E} \int_{K_e} \nabla \boldsymbol{\varphi}_i \cdot \nabla \boldsymbol{\varphi}_j = \sum_{e=1}^{N_E} \int_{K_e} \boldsymbol{f} \cdot \boldsymbol{\varphi}_j \quad \forall \boldsymbol{\varphi}_j \tag{4}$$

Appendix C: Example: Linear System of Equations

$$\sum_i u_i \underbrace{\sum_{e=1}^{N_E} \int_{K_e} \nabla \boldsymbol{\varphi}_i \cdot \nabla \boldsymbol{\varphi}_j}_{\mathbf{A}_{ij}} = \underbrace{\sum_{e=1}^{N_E} \int_{K_e} \boldsymbol{f} \cdot \boldsymbol{\varphi}_j}_{\boldsymbol{b}_j} \quad \forall \boldsymbol{\varphi}_j \tag{4}$$

Solving the finite element method consists of solving a linear system of equations:

$$\mathbf{A}\boldsymbol{x} = \boldsymbol{b}$$