PSI

Building Blocks for Finite Element computations in IPPL

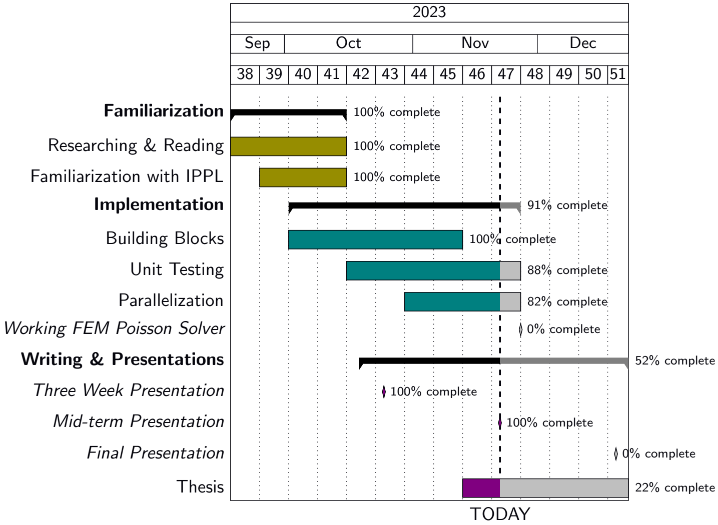
Mid-term Presentation

Lukas Bühler

Tuesday 21st November, 2023

Outline

Timeline (from 3-week presentation)



Outline

Transformation and Pullback

Transformation function (local ref. element $\hat{K}$ to global element K):

$$\mathbf{\Phi}_K : \hat{K} \mapsto K$$

We define the pullback $\mathbf{\Phi}_K^* f$ of a function f as

$$(\mathbf{\Phi}_K^* u)(\hat{\boldsymbol{x}}) := u(\mathbf{\Phi}_K(\hat{\boldsymbol{x}})), \quad \hat{\boldsymbol{x}} \in \hat{K}$$

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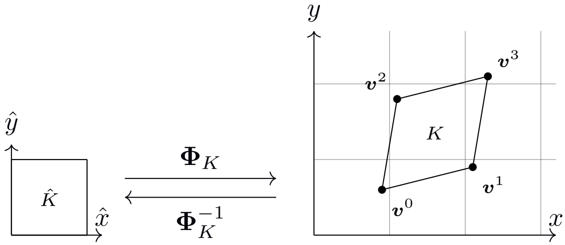
Affine Transformation Example

Affine Transformation: $\mathbf{\Phi}_K(\hat{\boldsymbol{x}}) = \mathbf{F}_K\hat{\boldsymbol{x}} + \boldsymbol{\tau}_K$



$$\text{with } \hat{\boldsymbol{x}} = \begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix},\ \boldsymbol{v}^i = \begin{pmatrix} \boldsymbol{v}^i_x \\ \boldsymbol{v}^i_y \end{pmatrix},\ \mathbf{F}_K = \begin{bmatrix} \boldsymbol{v}^1_x - \boldsymbol{v}^0_x & \boldsymbol{v}^2_x - \boldsymbol{v}^0_x \\ \boldsymbol{v}^1_y - \boldsymbol{v}^0_y & \boldsymbol{v}^2_y - \boldsymbol{v}^0_y \end{bmatrix},\ \boldsymbol{\tau}_K = \boldsymbol{v}^0$$

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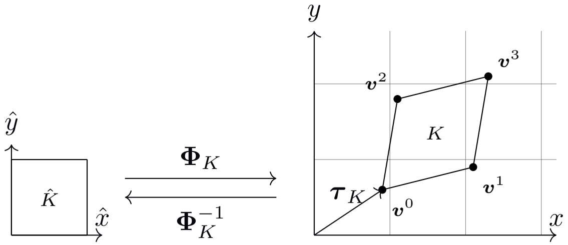

with $\hat{\boldsymbol{x}} = \begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix}, \; \boldsymbol{v}^i = \begin{pmatrix} \boldsymbol{v}_x^i \\ \boldsymbol{v}_y^i \end{pmatrix}, \; \mathbf{F}_K = \begin{bmatrix} \boldsymbol{v}_x^1 - \boldsymbol{v}_x^0 & \boldsymbol{v}_x^2 - \boldsymbol{v}_x^0 \\ \boldsymbol{v}_y^1 - \boldsymbol{v}_y^0 & \boldsymbol{v}_y^2 - \boldsymbol{v}_y^0 \end{bmatrix}, \; \boldsymbol{\tau}_K = \boldsymbol{v}^0$

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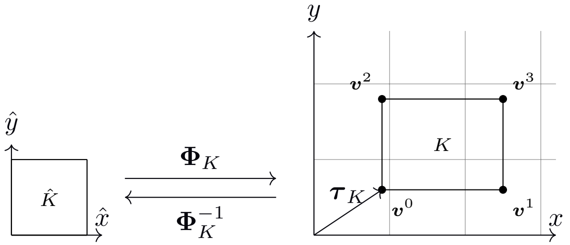

with $\hat{\boldsymbol{x}} = \begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix}$, $\boldsymbol{v}^i = \begin{pmatrix} \boldsymbol{v}_x^i \\ \boldsymbol{v}_y^i \end{pmatrix}$, $\mathbf{F}_K = \begin{bmatrix} \boldsymbol{v}_x^1 - \boldsymbol{v}_x^0 & 0 \\ 0 & \boldsymbol{v}_y^2 - \boldsymbol{v}_y^0 \end{bmatrix}$, $\boldsymbol{\tau}_K = \boldsymbol{v}^0$

Applying Pullback

Rewriting integrals over elements:

$$\int_K u(\boldsymbol{x})\ d\boldsymbol{x} = \int_{\hat{K}} (\boldsymbol{\Phi}_K^* u)(\hat{\boldsymbol{x}}) |\det \mathbf{D}\boldsymbol{\Phi}_K(\hat{\boldsymbol{x}})|\ d\hat{\boldsymbol{x}}$$
$$= \int_{\hat{K}} u(\boldsymbol{\Phi}_K(\hat{\boldsymbol{x}})) |\det \mathbf{D}\boldsymbol{\Phi}_K(\hat{\boldsymbol{x}})|\ d\hat{\boldsymbol{x}}$$

Rewriting gradients:

$$\boldsymbol{\Phi}_K^*(\nabla_{\boldsymbol{x}}\, u)(\hat{\boldsymbol{x}}) = (\mathbf{D}\boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}))^{-\top} \underbrace{(\nabla_{\hat{\boldsymbol{x}}}(\boldsymbol{\Phi}^* u))(\hat{\boldsymbol{x}})}_{=(\nabla_{\hat{\boldsymbol{x}}} u)(\boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}))}$$

with $\mathbf{S}^{-\top} := (\mathbf{S}^{-1})^\top = (\mathbf{S}^\top)^{-1}$

Jacobian of the Transformation (Example)

$$\mathbf{D}\boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}) = \left[\frac{\partial(\boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}))_i}{\partial \boldsymbol{x}_j}\right]_{i,j=1}^{d} = \begin{bmatrix} \boldsymbol{v}_x^1 - \boldsymbol{v}_x^0 & 0 \\ 0 & \boldsymbol{v}_y^2 - \boldsymbol{v}_y^0 \end{bmatrix}$$

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$$\mathbf{D\Phi}_K^{-1}(\hat{\boldsymbol{x}}) = \begin{bmatrix} \frac{1}{\boldsymbol{v}_x^1 - \boldsymbol{v}_x^0} & 0 \\ 0 & \frac{1}{\boldsymbol{v}_y^2 - \boldsymbol{v}_y^0} \end{bmatrix}$$

Outline

Assembly Algorithm (`evaluateAx`)

Input: $\boldsymbol{x}$

$\boldsymbol{z} \leftarrow \mathbf{0}$

for Element K in Mesh **do**

    // 1. Compute the Element matrix $\mathbf{A}_K$

    DOFs$_K \leftarrow \{4, 5, 8, 7\}$, DOFs$_{\hat{K}} \leftarrow \{0, 1, 2, 3\}$

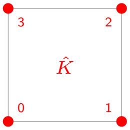
    ...

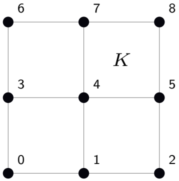
    // 2. Compute $\boldsymbol{z} = \mathbf{A}\boldsymbol{x}$ contribution with $\mathbf{A}_K$

    ...

end

return $\boldsymbol{z}$





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    $$(\mathbf{A}_K)_{i,j} = \int_K \nabla b_K^J(\boldsymbol{x}) \cdot \nabla b_K^I(\boldsymbol{x})\ d\boldsymbol{x}$$

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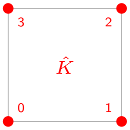

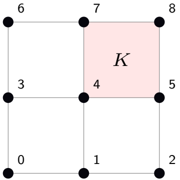

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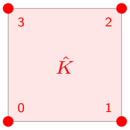

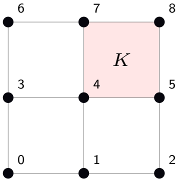

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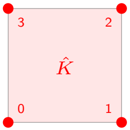

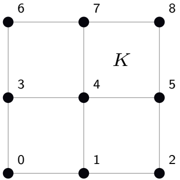

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  for $i, j \in \mathsf{DOFs}_{\hat{K}}$ **do**

$$(\mathbf{A}_K)_{i,j} \approx \sum_{k}^{N_{\mathsf{Int}}} \hat{\omega}_k (\mathbf{D\Phi}_K(\hat{\boldsymbol{q}}_k))^{-\top} \nabla \hat{b}^j(\hat{\boldsymbol{q}}_k) \cdot (\mathbf{D\Phi}(\hat{\boldsymbol{q}}_k))^{-\top} \nabla \hat{b}^i(\hat{q}_k) |\det \mathbf{D\Phi}_K(\hat{\boldsymbol{q}}_k)|$$

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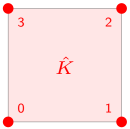

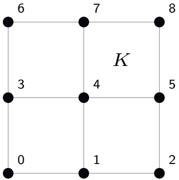

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    $I = \text{DOFs}_K[i]$, $J = \text{DOFs}_K[j]$

    $\boldsymbol{z}_I \leftarrow \boldsymbol{z}_I + (\mathbf{A}_K)_{i,j} \cdot \boldsymbol{x}_J$

  end

end

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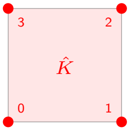

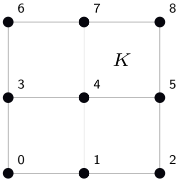

Assembly Algorithm (`evaluateLoadVector`)

Input: $\boldsymbol{x}$

$\boldsymbol{z} \leftarrow \mathbf{0}$

for Element K in Mesh **do**

    `// 1. Compute the Element vector` $\boldsymbol{b}_K$

    $\text{DOFs}_K \leftarrow \{4, 5, 8, 7\}$, $\text{DOFs}_{\hat{K}} \leftarrow \{0, 1, 2, 3\}$

    for $i \in \text{DOFs}_{\hat{K}}$ **do**

        $I = \text{DOFs}_K[i]$

        $$(\mathbf{b}_K)_i = \int_K f(x) b_K^I(x)\, dx$$

    end

    `// 2. Compute global right-hand side vector` $\boldsymbol{b}$ `contribution`

    for $i \in \text{DOFs}_{\hat{K}}$ **do**

        $I = \text{DOFs}_K[i]$,

        $\boldsymbol{b}_I \leftarrow \boldsymbol{b}_I + (\mathbf{b}_K)_i$

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  end

  `// 2. Compute global right-hand side vector` $\boldsymbol{b}$ `contribution`

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    end

end

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Outline

Quadrature

- Quadrature rule: Approximation of the definite integral of a function.
- Midpoint rule (Rectangle rule): $\int_a^b f(x)\ dx \approx (b-a)\, f\left(\frac{a+b}{2}\right)$

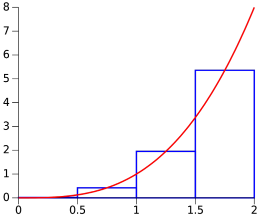

Figure: Mid-Riemann sum[1]

[1] By Qef - Own work, Public Domain, https://commons.wikimedia.org/w/index.php?curid=7081805

Gaussian Quadrature

n-point Gaussian quadrature rule yields exact results for polynomials of degree $2n-1$ or less with a suitable choice of nodes x_i and weights w_i, for $1 < i < n$.

$$\int_{-1}^{1} f(x)\, dx \approx \sum_{i=1}^{n} w_i\, f(x_i)$$

Examples:

- Gauss-Legendre Quadrature (x_i are the roots of the Legendre polynomial)
- Chebychev-Gauss Quadrature (x_i are the Chebychev nodes)
- Gauss-Jacobi Quadrature (x_i are the roots of the Jacobi polynomial)

Gauss-Jacobi quadrature

Jacobi polynomials are hypergeometric (a class of classical orthogonal polynomials).
Approximate integrals of the form:

$$\int_{-1}^{1} f(x)(1-x)^{\alpha}(1+x)^{\beta}\ dx$$

with $\alpha, \beta \geq -1$.
The following are special cases of the Gauss-Jacobi quadrature rule:

- Gauss-Legendre quadrature with $\alpha = \beta = 0$
- Chebychev-gauss quadrature with $|\alpha| = |\beta| = \frac{1}{2}$
- Gauss-Gegenbauer quadrature with $\alpha = \beta$

Orthogonal Polynomials and their Recurrence relation

- Recurrence relation: Equation that states that the n-th term of a sequence is equal to some combination of the previous terms.
  Example:

Orthogonal Polynomials and their Recurrence relation

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  Example: Fibonacci numbers: $F_n = F_{n-1} + F_{n-2}$

Orthogonal Polynomials and their Recurrence relation

- Recurrence relation: Equation that states that the n-th term of a sequence is equal to some combination of the previous terms. Example: Fibonacci numbers: $F_n = F_{n-1} + F_{n-2}$
- Orthogonal Polynomials: Sequence of polynomials such that any two different polynomials in the sequence are orthogonal under some inner product.
- Recurrence relation of classical orthogonal polynomials:

$$P_n(x) = (A_n x + B_n)P_{n-1}(x) + C_n P_{n-2}(x)$$

Gauss-Jacobi Implementation: Algorithm

Compared implementations of GSL[2], deal.II[3], LehrFEM++[4]

[2] https://www.gnu.org/software/gsl/doc/html/integration.html
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This algorithm follows the implementation in LehrFEM++

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Quadrature Implementation: Tensor Product

Tensor products are used to get the quadrature nodes and weights for a reference element.

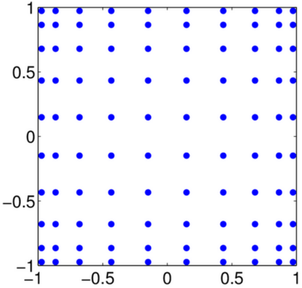

Figure: Gauss-Legendre quadrature 2D tensor product[5]

[5]Waves in Spatially-Disordered Neural Fields: A Case Study in Uncertainty Quantification

Outline

Plan for the (near) Future

- Finish Building Blocks: 3D
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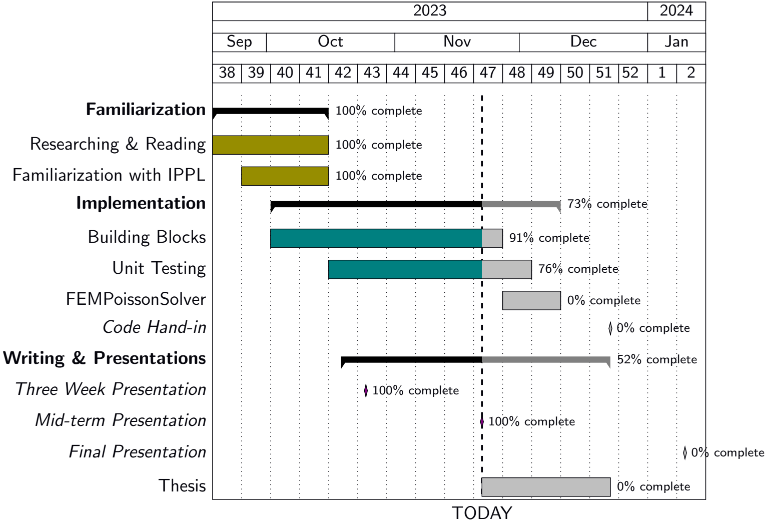
Updated Timeline



Appendix A: Global $\leftrightarrow$ Local Affine Transformations

- Local to Global: $\boldsymbol{x} = \boldsymbol{\Phi}_K(\hat{\boldsymbol{x}}) = \mathbf{F}_K\hat{\boldsymbol{x}} + \boldsymbol{\tau}_K$
- Global to Local: $\hat{\boldsymbol{x}} = \boldsymbol{\Phi}_K^{-1}(\boldsymbol{x}) = \mathbf{F}_K^{-1}(\boldsymbol{x} - \boldsymbol{\tau}_K)$