A Performance and Energy Study of the Hyperbolic PDE Solver Engine ExaHyPE

Master's Thesis in Computational Science and Engineering

Fabian Güra
Department of Informatics
Technische Universität München

September 2016

Supervisors: Univ.-Prof. Dr. Michael Bader
Dr. Tobias Weinzierl
Advisor: Dr. Vasco Varduhn

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Abstract

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Chapter 1

Introduction

- Challenges of exascale
- The ExaHyPE project (numerics, resilience, profiling) as an answer
- On the importance of profiling and performance measuring

Chapter 2

Theory

2.1 A D-dimensional ADER-DG scheme with MUSCL-Hancock a-posteriori subcell limiting for non-linear hyperbolic conservation laws

Arbitrary High Order Derivatives Discontinuous Galerkin (ADER-DG)

2.1.1 Notation

We use vector notation whenever possible. Advantage: Complete derivation, direct conversion to code.

2.1.2 PDE

Task: Solve the PDE

$$\frac{\partial}{\partial t}\left[\boldsymbol{u}\right]_v + \frac{\partial}{\partial x_d}\left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd} = \left[\boldsymbol{S}(\boldsymbol{u})\right]_v \text{ on } \boldsymbol{\Omega}\times(0,T) \tag{2.1}$$

with initial conditions

$$\left[\boldsymbol{u}(\boldsymbol{x},0)\right]_v = \left[\boldsymbol{u}_0(\boldsymbol{x})\right]_v\ \forall \boldsymbol{x}\in\boldsymbol{\Omega}, \tag{2.2}$$

and boundary conditions

$$\left[\boldsymbol{u}(\boldsymbol{x},t)\right]_v = \left[\boldsymbol{u}_B(\boldsymbol{x},t)\right]_v\ \forall \boldsymbol{x}\in\partial\boldsymbol{\Omega}, t\in(0,T), \tag{2.3}$$

for all $v\in\mathcal{V}$, where we define the index set $\mathcal{V}=\{1,2,\ldots,V\}$ for V being the number of quantities that describe the state of the physical system, $\boldsymbol{\Omega}\subset\mathbb{R}^D$ is the spatial domain, D the number of space dimensions and $[0,T]$ a time interval. The function $\boldsymbol{F}:\mathbb{R}^V\to\mathbb{R}^{V\times D}, \boldsymbol{u}\mapsto\boldsymbol{F}(\boldsymbol{u})=\left[\boldsymbol{f}_1(\boldsymbol{u}),\boldsymbol{f}_2(\boldsymbol{u}),\ldots,\boldsymbol{f}_D(\boldsymbol{u})\right]$ is called the flux function.

For the problem to be hyperbolic we require that all Jacobian matrices $\boldsymbol{A}_d(\boldsymbol{u})$, $d \in \{1, 2, \ldots, D\} := \mathcal{D}$, defined as

$$[\boldsymbol{A}_d]_{ij} = \frac{\partial\, [\boldsymbol{f}_d]_i}{\partial u_j}, \tag{2.4}$$

have D real eigenvalues in each admissible state $\boldsymbol{u}$.

2.1.3 Mesh

Let $\mathcal{K}_h$ be a quadrilateral partition of $\boldsymbol{\Omega}$, i.e.

$$K \cap J = \emptyset \forall K, J \in \mathcal{K}_h, K \neq J, \tag{2.5}$$

$$\bigcup_{K \in \mathcal{K}_h} K = \boldsymbol{\Omega}. \tag{2.6}$$

For the index set $\mathcal{I} := \{0, 1, \ldots, I-1\}$ let $\{t_i\}_{i \in \mathcal{I}}$ be an I-fold partition of the time interval $[0, T]$ such that

$$0 = t_0 < t_1 < \ldots < t_I = T. \tag{2.7}$$

For $i \in \mathcal{I}$ we furthermore define

$$\Delta t_i = t_{i+1} - t_i, \tag{2.8}$$

so that the interval $[t_i, t_{i+1}]$ can be written as $[t_i, t_i + \Delta t_i]$.

2.1.4 Weak formulation

Let $L^2(\boldsymbol{\Omega})^V$ be the space of vector-valued, square-integrable functions on $\boldsymbol{\Omega}$, i.e.

$$L^2(\boldsymbol{\Omega})^V = \left\{ \boldsymbol{w} : \Omega \to \mathbb{R}^V \mid \int_{\Omega} \|\boldsymbol{w}\|^2 \, d\boldsymbol{x} < \infty \right\}. \tag{2.9}$$

Let $\boldsymbol{w} \in L^2(\boldsymbol{\Omega})^V$ be a spatial test function. Multiplication of the original PDE (2.1) and integration over a space-time cell $K \times [t_i, t_i + \Delta t_i]$ yields a weak, element local formulation of the problem

$$\begin{aligned} &\int_{t_i}^{t_i+\Delta t_i} \int_K \frac{\partial}{\partial t} [\boldsymbol{u}]_v \, [\boldsymbol{w}]_v \, d\boldsymbol{x}\, dt + \int_{t_i}^{t_i+\Delta t_i} \int_K \frac{\partial}{\partial x_d} \left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd} [\boldsymbol{w}]_v \, d\boldsymbol{x}\, dt = \\ &\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{S}(\boldsymbol{u})\right]_v [\boldsymbol{w}]_v \, d\boldsymbol{x}\, dt, \end{aligned} \tag{2.10}$$

which we require to hold for all $v \in \mathcal{V}$, $\boldsymbol{w} \in L^2(\boldsymbol{\Omega})^V$, $K \in \mathcal{K}_h$ and $i \in \mathcal{I}$.

Integration by parts of the spatial integral in the second term yields

$$\begin{aligned}&\int_K \frac{\partial}{\partial x_d} \left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd} \left[\boldsymbol{w}\right]_v \, d\boldsymbol{x} = \\ &\int_K \frac{\partial}{\partial x_d} \Big(\left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd} \left[\boldsymbol{w}\right]_v \Big) \, d\boldsymbol{x} - \int_K \left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd} \frac{\partial}{\partial x_d} \left[\boldsymbol{w}\right]_v \, d\boldsymbol{x}.\end{aligned} \tag{2.11}$$

Application of the divergence theorem to the first term on the right-hand side of (2.11) yields

$$\int_K \frac{\partial}{\partial x_d} \Big(\left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd} \left[\boldsymbol{w}\right]_v \Big) \, d\boldsymbol{x} = \int_{\partial K} \left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd} \left[\boldsymbol{w}\right]_v \left[\boldsymbol{n}\right]_d \, ds(\boldsymbol{x}), \tag{2.12}$$

where $\boldsymbol{n} \in \mathbb{R}^D$ is the unit-length, outward-pointing normal vector at a point $\boldsymbol{x}$ on the surface of K, which we denote by ∂K.

Inserting eqs. (2.11) and (2.12) into eq. (2.10) yields the following weak, element-local formulation of the original equation (2.1):

$$\begin{aligned}&\int_{t_i}^{t_i+\Delta t_i} \int_K \frac{\partial}{\partial t} \left[\boldsymbol{u}\right]_v \left[\boldsymbol{w}\right]_v \, d\boldsymbol{x}\, dt - \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd} \frac{\partial}{\partial x_d} \left[\boldsymbol{w}\right]_v \, d\boldsymbol{x}\, dt + \\ &\int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd} \left[\boldsymbol{w}\right]_v \left[\boldsymbol{n}\right]_d \, ds(\boldsymbol{x})\, dt = \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{S}(\boldsymbol{u})\right]_v \left[\boldsymbol{w}\right]_v \, d\boldsymbol{x}\, dt.\end{aligned} \tag{2.13}$$

Again we require the weak formulation to hold for all $v \in \mathcal{V}$, $\boldsymbol{w} \in L^2(\boldsymbol{\Omega})^V$, $K \in \mathcal{K}_h$ and $i \in \mathcal{I}$.

2.1.5 Restriction to finite-dimensional function spaces

To discretize eq. (2.13) we need to impose the restriction that both test and ansatz functions come from a finite-dimensional space. First, let $\mathbb{Q}_N(K)^V$ and $\mathbb{Q}_N(K \times [t_i, t_i + \Delta t_i])^V$ be the space of vector-valued, multivariate polynomials of degree less or equal N in each variable on K and $K \times [t_i, t_i + \Delta t_i]$, respectively. We then make the following choices:

- For spatial functions we restrict ourselves to

$$\mathbb{W}_h = \left\{ \boldsymbol{w}_h \in L^2(\boldsymbol{\Omega})^V : \boldsymbol{w}_h|_K := \boldsymbol{w}_h^K \in \mathbb{Q}_N(K)^V \, \forall K \in \mathcal{K}_h \right\}. \tag{2.14}$$

- For space-time functions we restrict ourselves to

$$\begin{aligned}\tilde{\mathbb{W}}_h^i = \Big\{ &\tilde{\boldsymbol{w}}_h^i \in L^2 \left(\boldsymbol{\Omega} \times [t_i, t_i + \Delta t_i] \right) \mid \\ &\tilde{\boldsymbol{w}}_h^i \Big|_K := \tilde{\boldsymbol{w}}_h^{K,i} \in \mathbb{Q}_N \left(K \times [t_i, t_i + \Delta t_i] \right) \forall K \in \mathcal{K}_h \Big\}\end{aligned} \tag{2.15}$$

  for all $i \in \mathcal{I}$.

Replacing $\boldsymbol{w}$ by $\boldsymbol{w}_h \in \mathbb{W}_h$ and $\boldsymbol{u}$ by $\tilde{\boldsymbol{u}}_h^i \in \tilde{\mathbb{W}}_h^i$ in eq. (2.13) yields a finite-dimensional approximation of the weak formulation,

$$\int_{t_i}^{t_i+\Delta t_i} \int_K \frac{\partial}{\partial t} \left[\tilde{\boldsymbol{u}}_h^{K,i}\right]_v \left[\boldsymbol{w}_h^K\right]_v \, d\boldsymbol{x}\, dt - \int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{F}(\tilde{\boldsymbol{u}}_h^{K,i})\right]_{vd} \frac{\partial}{\partial x_d} \left[\boldsymbol{w}_h^K\right]_v \, d\boldsymbol{x}\, dt +$$
$$\int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{\mathcal{G}}(\tilde{\boldsymbol{u}}_h^{K,i}, \tilde{\boldsymbol{u}}_h^{K^+i}, \boldsymbol{n})\right]_v \left[\boldsymbol{w}_h^K\right]_v \, ds(\boldsymbol{x})\, dt =$$
$$\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{S}(\tilde{\boldsymbol{u}}_h^{K,i})\right]_v \left[\boldsymbol{w}_h^K\right]_v \, d\boldsymbol{x}\, dt, \tag{2.16}$$

which now has to hold for all $\boldsymbol{w}_h \in \mathbb{W}_h$, $K \in \mathcal{K}_h$ and $i \in \{0, 1, \ldots, I-1\}$. Since for a cell $K \in \mathcal{K}_h$ and one of its Voronoi neighbors $K' \in \mathcal{V}(K)$ one has in general

$$\tilde{\boldsymbol{u}}_h^{K,i}(\boldsymbol{x}^*) \neq \tilde{\boldsymbol{u}}_h^{K'i}(\boldsymbol{x}^*),\ \boldsymbol{x}^* \in K \cap K', \tag{2.17}$$

i.e. $\tilde{\boldsymbol{u}}_h^i$ is double-valued at the interface between K and K', in order to compute the surface integral we need to introduce the numerical flux function $\boldsymbol{\mathcal{G}}(\tilde{\boldsymbol{u}}_h^{K,i}, \tilde{\boldsymbol{u}}_h^{K'i}, \boldsymbol{n})$. The numerical flux at a position $\boldsymbol{x}^* \in K \cap K'$ on the interface is obtained by (approximately) solving a Riemann problem in normal direction.

Riemann problem: Let $\boldsymbol{x}^*$ be a point on interface ∂K between a cell K and its Voronoi K' in $\boldsymbol{x}$ and let $\boldsymbol{n}$ be the outward pointing unit normal vector at this point. Then to obtain the numerical flux we need to solve the initial boundary value problem ("Riemann problem")

$$\frac{\partial}{\partial t} \left[\boldsymbol{g}\right]_v + \sum_{d=1}^{D} \frac{\partial}{\partial x_d} \left[\boldsymbol{F}(\boldsymbol{g})\right]_{vd} \left[\boldsymbol{n}\right]_d = 0 \tag{2.18}$$

along the line $\boldsymbol{x} = \boldsymbol{x}^* + \alpha \boldsymbol{n}$ for $\alpha \in \mathbb{R}$ with discontinuous initial conditions

$$\boldsymbol{g}(\boldsymbol{x}^* + \alpha \boldsymbol{n}, 0) = \begin{cases} \tilde{\boldsymbol{u}}_h^{K,i}\Big|_{\boldsymbol{x}^*} & \text{if } \alpha < 0 \\ \tilde{\boldsymbol{u}}_h^{K',i}\Big|_{\boldsymbol{x}^*} & \text{if } \alpha > 0. \end{cases} \tag{2.19}$$

We then evaluate the similarity solution $\tilde{\boldsymbol{g}}(\alpha/t)$ to define

$$\left[\boldsymbol{\mathcal{G}}\left(\tilde{\boldsymbol{u}}_h^{K,i}, \tilde{\boldsymbol{u}}_h^{K',i}, \boldsymbol{n}\right)\right]_v := \left[\tilde{\boldsymbol{g}}\big|_0\right]_v. \tag{2.20}$$

TODO: Overview state of the art solver.

Integration by parts in time of the first term of eq. (2.16) and noting that $\boldsymbol{w}_h$ is constant in time yields the following one-step update scheme for the cell-local time-discrete solution $\tilde{\boldsymbol{u}}_h^{K,i}$:

$$\begin{aligned}\int_K \left[\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i+\Delta t_i}\right]_v \left[\boldsymbol{w}_h^K\right]_v \, d\boldsymbol{x} = \int_K \left[\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i}\right]_v \left[\boldsymbol{w}_h^K\right]_v \, d\boldsymbol{x} + \\ \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{u}}_h^{K,i})\right]_{vd} \frac{\partial}{\partial x_d} \left[\boldsymbol{w}_h^K\right]_v \, d\boldsymbol{x}\, dt - \\ \int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{\mathcal{G}}(\tilde{\boldsymbol{u}}_h^{K,i}, \tilde{\boldsymbol{u}}_h^{K^+i}, \boldsymbol{n})\right]_v \left[\boldsymbol{w}_h^K\right]_v \, ds(\boldsymbol{x})\, dt + \\ \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{S}(\tilde{\boldsymbol{u}}_h^{K,i})\right]_v \left[\boldsymbol{w}_h^K\right]_v \, d\boldsymbol{x}\, dt.\end{aligned} \tag{2.21}$$

Again we require eq. (2.21) to hold for all $v \in \mathcal{V}$, $\boldsymbol{w}_h \in \mathbb{W}_h$, $K \in \mathcal{K}_h$ and $i \in \mathcal{I}$.

Problem: We only have $\tilde{\boldsymbol{u}}_h^i\Big|_t$ at the discrete time steps $t \in \{t_i, t_i + \Delta t_i\}$, not within the open interval, i.e. for $t \in (t_i, t_i + \Delta t_i)$.

Idea: Replace $\tilde{\boldsymbol{u}}_h$ in $K \times (t_i, t_i + \Delta t_i)$ by an approximation $\tilde{\boldsymbol{q}}_h^i \in \tilde{\mathbb{W}}_h^i$ which we call space-time predictor.

2.1.6 Space-time predictor

To derive a procedure to compute the space-time predictor $\tilde{\boldsymbol{q}}_h^i \in \tilde{\mathbb{W}}_h^i$ we again start from the original PDE (2.1), but this time we do not use a spatial test function $\boldsymbol{w}_h \in \mathbb{W}_h$, but a space-time test function $\tilde{\boldsymbol{w}}_h^i \in \tilde{\mathbb{W}}_h^i$. If we furthermore replace the solution $\boldsymbol{u}$ by the the space-time predictor $\tilde{\boldsymbol{q}}_h^i \in \tilde{\mathbb{W}}_h^i$, integrate over the space-time element $K \times [t_i, t_i + \Delta t_i]$ and apply the divergence theorem analogously to eq. (2.12) we obtain the following relation:

$$\begin{aligned}\int_{t_i}^{t_i+\Delta t_i} \int_K \frac{\partial}{\partial t} \left[\tilde{\boldsymbol{q}}_h^{K,i}\right]_v \left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_v \, d\boldsymbol{x}\, dt - \\ \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{q}}_h^{K,i})\right]_{vd} \frac{\partial}{\partial x_d} \left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_v \, d\boldsymbol{x}\, dt + \\ \int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{\mathcal{G}}\left(\tilde{\boldsymbol{q}}_h^{K,i}, \tilde{\boldsymbol{q}}_h^{K^+i}, \boldsymbol{n}\right)\right]_v \left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_v \, ds(\boldsymbol{x})\, dt = \\ \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{S}\left(\tilde{\boldsymbol{q}}_h^{K,i}\right)\right]_v \left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_v \, d\boldsymbol{x}\, dt.\end{aligned} \tag{2.22}$$

We require eq. (2.22) to hold for all $v \in \mathcal{V}$, $\tilde{\boldsymbol{w}}_h^i \in \tilde{\mathbb{W}}_h^i$, $K \in \mathcal{K}_h$ and $i \in \mathcal{I}$.

The assumption that the solution is balanced, i.e. that there is no net inflow or outflow for cell $K \in \mathcal{K}_h$ allows us to drop the third term. Together with integration by parts in time of the first term this yields

$$\int_K \left[\tilde{\boldsymbol{q}}_h^{K,i}\Big|_{t_i+\Delta t_i} \right]_v \left[\tilde{\boldsymbol{w}}_h^{K,i}\Big|_{t_i+\Delta t_i} \right]_v d\boldsymbol{x} - \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\tilde{\boldsymbol{q}}_h^{K,i} \right]_v \frac{\partial}{\partial t} \left[\tilde{\boldsymbol{w}}_h^{K,i} \right]_v d\boldsymbol{x}\, dt = \int_K \left[\tilde{\boldsymbol{q}}_h^{K,i}\Big|_{t_i} \right]_v \left[\tilde{\boldsymbol{w}}_h^{K,i}\Big|_{t_i} \right]_v d\boldsymbol{x} + \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{q}}_h^{K,i}) \right]_{vd} \frac{\partial}{\partial x_d} \left[\tilde{\boldsymbol{w}}_h^{K,i} \right]_v d\boldsymbol{x}\, dt + \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{S}\left(\tilde{\boldsymbol{q}}_h^{K,i} \right) \right]_v \left[\tilde{\boldsymbol{w}}_h^{K,i} \right]_v d\boldsymbol{x}\, dt, \tag{2.23}$$

which we require to hold for all $v \in \mathcal{V}$, $\tilde{\boldsymbol{w}}_h^i \in \tilde{\mathbb{W}}_h^i$, $K \in \mathcal{K}_h$ and $i \in \mathcal{I}$. Together with the initial condition

$$\tilde{\boldsymbol{q}}_h^{K,i}\Big|_{t_i} = \tilde{\boldsymbol{u}}_h^{K}\Big|_{t_i} \tag{2.24}$$

and an initial guess

$$\tilde{\boldsymbol{q}}_h^{K,i}\Big|_{t} = \tilde{\boldsymbol{u}}_h^{K}\Big|_{t_i} \ \forall t \in [t_i, t_i + \Delta t_i] \tag{2.25}$$

this relation can be used as a fixed-point iteration to find the cell-local space-time predictor $\tilde{\boldsymbol{q}}_h^{K,i}$.

In the following two sections we will introduce mappings from spatial elements K and space-time elements $K \times [t_i, t_i + \Delta t_i]$ to spatial and space-time reference cells and orthogonal bases for the spaces $\mathbb{W}_h$ and $\tilde{\mathbb{W}}_h^i$. We will then insert these results into eq. (2.23) and derive a fully-discrete iterative method to compute the cell-local space-time predictor $\tilde{\boldsymbol{q}}_h^{K,i}$.

2.1.7 Mappings

Let $\hat{K} = [0,1]^D$ be the spatial reference element and $\boldsymbol{\xi} \in \hat{K}$ be a point in the reference element. Let $[0,1]$ be the reference time interval and $\tau \in [0,1]$ be a point in time in reference time.

We can then introduce the following mappings:

Spatial mappings: Let $K \in \mathcal{K}_h$ be a cell in global coordinates with extent $\Delta \boldsymbol{x}^K$ and "lower-left corner" $\boldsymbol{P}_K$, more precisely that is

$$\left[\Delta \boldsymbol{x}^K \right]_d = \max_{\boldsymbol{x} \in K} [\boldsymbol{x}]_d - \min_{\boldsymbol{x} \in K} [\boldsymbol{x}]_d \tag{2.26}$$

and

$$[\boldsymbol{P}_K]_d = \min_{\boldsymbol{x} \in K} [\boldsymbol{x}]_d \tag{2.27}$$

for $d \in \mathcal{V}$. We can then define a mapping

$$\boldsymbol{\mathcal{X}}_K : \hat{K} \to K, \boldsymbol{\xi} \mapsto \boldsymbol{\mathcal{X}}_K(\boldsymbol{\xi}) = \boldsymbol{x} \tag{2.28}$$

via the relation

$$[\boldsymbol{x}]_d = \left[\boldsymbol{\mathcal{X}}_K(\boldsymbol{\xi})\right]_d = [\boldsymbol{P}_K]_d + [\Delta \boldsymbol{x}]_d \left[\boldsymbol{\xi}\right]_d \tag{2.29}$$

for $v \in \mathcal{V}$ (i.e. no summation on v) and for all $\boldsymbol{x} \in K$, $\boldsymbol{\xi} \in \hat{K}$ and $K \in \mathcal{K}_h$.

Temporal mappings: Let $(t_i, t_i + \Delta t_i), i \in \mathcal{I}$ be an interval in global time. The mapping

$$\mathcal{T}_i : [0,1] \to [t_i, t_i + \Delta t_i], \tau \mapsto \mathcal{T}_i(\tau) = t_i + \Delta t_i \tau = t \tag{2.30}$$

maps a point in reference time $\tau \in [0,1]$ to a point in global time $t \in [t_i, t_i + \Delta t_i]$ for all $i \in \mathcal{I}$.

The inverse mappings, the Jacobian matrices and the Jacobi determinants of the mappings are given in the following:

Spatial mappings: The inverse spatial mappings

$$\boldsymbol{\mathcal{X}}_K^{-1} : K \to \hat{K}, \boldsymbol{x} \mapsto \boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x}) = \boldsymbol{\xi} \tag{2.31}$$

are defined via the relation

$$\left[\boldsymbol{\xi}\right]_d = \left[\boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x})\right]_d = \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_d} \left([\boldsymbol{x}]_d - [\boldsymbol{P}_K]_d\right) \tag{2.32}$$

for $v \in \mathcal{V}$ and for all $\boldsymbol{\xi} \in \hat{K}$, $\boldsymbol{x} \in K$ and $K \in \mathcal{K}_h$. The Jacobian of $\boldsymbol{\mathcal{X}}_K$ is found to be

$$\left[\frac{\partial \boldsymbol{\mathcal{X}}_K}{\partial \boldsymbol{\xi}}\right]_{dd'} = \frac{\partial \left[\boldsymbol{\mathcal{X}}_K\right]_d}{\partial \xi_{d'}} = \left[\Delta \boldsymbol{x}^K\right]_d \delta_{dd'}, \tag{2.33}$$

where $d, d' \in \mathcal{D}$ (i.e. no summation on d) and for all $K \in \mathcal{K}_h$. As usual $\delta_{dd'}$ denotes the Kronecker delta defined as

$$\delta_{dd'} = \begin{cases} 0 & \text{if } d \neq d' \\ 1 & \text{if } d = d'. \end{cases} \tag{2.34}$$

The Jacobi determinant of $\boldsymbol{\mathcal{X}}_K$ for $K \in \mathcal{K}_h$ then simply is

$$J_{\boldsymbol{\mathcal{X}}_K} = \| \frac{\partial \boldsymbol{\mathcal{X}}_K}{\partial \boldsymbol{\xi}} \| = \prod_{d=1}^{D} \left[\Delta \boldsymbol{x}^K\right]_d, \tag{2.35}$$

i.e. the determinant is constant for all $\boldsymbol{x} \in K$.

Temporal mappings: The inverse temporal mappings are given as

$$\mathcal{T}_i^{-1} : [t_i, t_i + \Delta t_i] \to [0,1], t \mapsto \mathcal{T}_i^{-1}(t) = \frac{t - t_i}{\Delta t_i} = \tau \tag{2.36}$$

for all $\tau \in [0,1]$, $t \in [t_i, t_i + \Delta t_i]$ and $i \in \mathcal{I}$. In the trivial case of a one-dimensional mapping the Jacobian of $\mathcal{T}_i$ is a scalar which in turn is its own determinant. One finds

$$\frac{d\mathcal{T}_i}{\partial \tau} = \Delta t_i = J_{\mathcal{T}_i} \tag{2.37}$$

which again is constant for all $t \in [t_i, t_i + \Delta t_i]$ for a fixed $i \in \mathcal{I}$.

2.1.8 Orthogonal bases for the finite-dimensional spatial and space-time function spaces

Lagrange interpolation

Let $f \in \mathbb{Q}_N([0,1])$ be a polynomial of degree N and for the index set $\mathcal{N} := \{0, 1, \ldots, N\}$ let $\{\hat{\xi}_n\}_{n \in \mathcal{N}}$ be a set of distinct nodes in $[0,1]$. The the Lagrange interpolation of f,

$$\hat{f}(\xi) = \sum_{n=0}^{N} L_n(\xi) f(\xi_n) \tag{2.38}$$

with Lagrange functions

$$L_n(\xi) = \prod_{m=0, m \neq n}^{N} \frac{\xi - \hat{\xi}_m}{\hat{\xi}_n - \hat{\xi}_m} \tag{2.39}$$

is exact, i.e.

$$f(\xi) = \hat{f}(\xi) \, \forall \xi \in [0,1]. \tag{2.40}$$

Since every polynomial $f \in \mathbb{Q}_N([0,1])$ can be represented as a linear combination of the Legendre polynomials L_n the set of functions $\{L_n\}_{n \in \mathcal{N}}$ is a basis of $Q_N([0,1])$.

The following observation is an important property of the Lagrange polynomials:

$$L_n(\hat{\xi}_{n'}) = \delta_{nn'}, \tag{2.41}$$

i.e. at each node $\hat{\xi}_n$ only L_n has value 1 and all other polynomials evaluate to 0.

Legendre polynomials and Gauss-Legendre integration

Let $P_0 : [-1,1] \to \mathbb{R}, \xi \mapsto 1$ and $P_1 : [-1,1] \to \mathbb{R}, \xi \mapsto \xi$ be the zeroth and the first Legendre polynomial, respectively. Then the $N+1$-st Legendre polynomial can be defined via the following recurrence relation:

$$P_{N+1}(\xi) = \frac{1}{N+1}\left((2N+1)P_N(\xi) - nP_{N-1}(\xi)\right). \tag{2.42}$$

Let $\{\tilde{\xi}_n\}_{n\in\mathcal{N}}$ be the roots of the $N+1$-st Legendre polynomial L_{N+1}. Then $\{\hat{\xi}_n\}_{n\in\mathcal{N}}$ with

$$\hat{\xi}_n = \frac{1}{2}(\tilde{\xi}_n + 1) \tag{2.43}$$

are the roots of the $N+1$-st Legendre polynomial linearly mapped to the interval $(0,1)$. In conjunction with a set of suitable weights $\{\hat{\omega}_n\}_{n\in\mathcal{N}}$ Gauss-Legendre integration can be used to integrate polynomials of degree up to $2N+1$ over the integral $[0,1]$ exactly, i.e.

$$\int_0^1 f(\xi)\, d\xi = \sum_{n=0}^{N} \hat{\omega}_n f(\hat{\xi}_n)\, \forall f \in \mathbb{Q}_{2N+1}\left([0,1]\right). \tag{2.44}$$

A script on how to find the weights $\{\hat{\xi}_n\}_{n\in\mathcal{N}}$ can be found in appendix XXX.

1d basis functions

Let $\{\hat{\psi}_n\}_{n\in\mathcal{N}}$ be the set of $N+1$ Lagrange polynomials with nodes at the roots of the $N+1$-st Legendre polynomial linearly mapped to the interval $[0,1]$, i.e.

$$\hat{\psi}_n(x) = \sum_{n'=0}^{N} \frac{x - \hat{x}_{n'}}{\hat{x}_n - \hat{x}_{n'}} \tag{2.45}$$

for $n \in \mathcal{N}$. Since $\{\hat{\psi}_n\}_{n\in\mathcal{N}}$ are Lagrange polynomials and the roots $\{\hat{x}_n\}_{n\in\mathcal{N}}$ are distinct the set is a basis of $\mathbb{Q}_N([0,1])$. Since furthermore

$$\left\langle \hat{\psi}_n, \hat{\psi}_m \right\rangle_{L^2\left([0,1]\right)} = \int_0^1 \hat{\psi}_n(x)\hat{\psi}_m(x)\, d\boldsymbol{x} = \sum_{n'=0}^{N} \hat{w}'_n \hat{\psi}_n(\hat{x}_{n'})\hat{\psi}_m(\hat{x}_{n'}) = \hat{w}_n \delta_{mn} \tag{2.46}$$

for all $m, n \in \mathcal{N}$ (i.e. no summation over n), the set is even an orthogonal basis of $\mathbb{Q}_N([0,1])$ with respect to the L^2-scalar product as defined above. In this derivation we used the fact that $\hat{\psi}_n\hat{\psi}_m$ has degree $2N$ and that Gauss-Legendre integration with $N+1$ nodes is exact for polynomials up to degree $2N+1$.

Scalar-valued basis functions on the spatial reference element

For the vector-valued index set $\boldsymbol{\mathcal{N}} := \{0, 1, \ldots, N\}^D$ let us define the set of scalar-valued spatial basis functions $\{\hat{\phi}_{\boldsymbol{n}}\}_{\boldsymbol{n}\in\boldsymbol{\mathcal{N}}}$ on $\hat{K} := [0,1]^D$ as

$$\hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi}) = \prod_{d=1}^{D} \hat{\psi}_{[\boldsymbol{n}]_d}([\boldsymbol{\xi}]_d) = \hat{\psi}_{[\boldsymbol{n}]_d}([\boldsymbol{\xi}]_d), \tag{2.47}$$

i.e. $\{\hat{\phi}_{\boldsymbol{n}}\}_{\boldsymbol{n}\in\boldsymbol{\mathcal{N}}}$ is the tensor product of $\{\hat{\psi}_n\}_{n\in\mathcal{N}}$ and as such it is a basis of $\mathbb{Q}([0,1]^D) = \mathbb{Q}(\hat{K})$. If we define

$$\left[\hat{\boldsymbol{\xi}}_{\boldsymbol{n}}\right]_d = \hat{\xi}_{[\boldsymbol{n}]_d} \tag{2.48}$$

and

$$\prod_{d=1}^{D} \hat{\omega}_{[\boldsymbol{n}]_d}, \tag{2.49}$$

for all $d \in \mathcal{V}$ and $\boldsymbol{n} \in \boldsymbol{\mathcal{N}}$, we furthermore observe that the basis is orthogonal with respect to the L^2-scalar product, since

$$\begin{gathered}\left\langle \hat{\phi}_{\boldsymbol{n}}, \hat{\phi}_{\boldsymbol{m}} \right\rangle_{L^2(\hat{K})} = \int_{\hat{K}} \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi})\hat{\phi}_{\boldsymbol{m}}(\boldsymbol{\xi})\, d\boldsymbol{\xi} = \\ \sum_{\boldsymbol{n}'\in\boldsymbol{\mathcal{N}}} \left(\hat{\omega}_{\boldsymbol{n}'}\hat{\phi}_{\boldsymbol{n}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{n}'})\hat{\phi}_{\boldsymbol{m}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{n}'})\right) = \hat{\omega}_{\boldsymbol{n}}\delta_{\boldsymbol{nm}}\end{gathered} \tag{2.50}$$

for all $\boldsymbol{n}, \boldsymbol{m} \in \boldsymbol{\mathcal{N}}$. The natural extensions of the Kronecker delta for vector-valued indices is defined as follows:

$$\delta_{\boldsymbol{nm}} = \prod_{d=1}^{D} \delta_{[\boldsymbol{n}]_d[\boldsymbol{m}]_d} = \delta_{[\boldsymbol{n}]_d[\boldsymbol{m}]_d}. \tag{2.51}$$

Scalar-valued basis functions on the space-time reference element

Analogously to the procedure illustrated above for the spatial reference element $\hat{K}$ we can define a basis $\{\hat{\theta}_{\boldsymbol{n}l}\}_{\boldsymbol{n}\in\boldsymbol{\mathcal{N}}, l\in\mathcal{N}}$ of $\mathbb{Q}_N(\hat{K} \times [0,1])$ on the reference space-time element $\hat{K} \times [0,1]$ as

$$\hat{\theta}_{\boldsymbol{n}l}(\boldsymbol{\xi}, \tau) = \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi})\hat{\psi}_l(\tau), \tag{2.52}$$

which again is orthogonal, since

$$\left\langle \hat{\theta}_{\boldsymbol{n}l}, \hat{\theta}_{\boldsymbol{m}k} \right\rangle_{L^2(\hat{K}\times[0,1])} = \int_0^1 \int_{\hat{K}} \hat{\theta}_{\boldsymbol{n}l}\hat{\theta}_{\boldsymbol{m}k}\, d\boldsymbol{\xi}\, d\tau = \hat{\omega}_{\boldsymbol{n}}\hat{\omega}_l\delta_{\boldsymbol{nm}}\delta_{lk} \tag{2.53}$$

for all $\boldsymbol{n}, \boldsymbol{m} \in \boldsymbol{\mathcal{N}}$ and $l, k \in \mathcal{N}$.

Vector-valued basis functions on the spatial reference element

If we define $\{\hat{\boldsymbol{\phi}}_{\boldsymbol{n}v}\}_{\boldsymbol{n}\in\boldsymbol{\mathcal{N}},v\in\mathcal{V}}$ as

$$\hat{\boldsymbol{\phi}}_{\boldsymbol{n}v} = \hat{\phi}_{\boldsymbol{n}}\boldsymbol{e}_v, \tag{2.54}$$

where $\boldsymbol{e}_v$ is the v-th unit vector, i.e.

$$[\boldsymbol{e}_v]_{v'} = \delta_{vv'} \tag{2.55}$$

for $v, v' \in \mathcal{V}$. Since

$$\begin{aligned} &\left\langle \hat{\boldsymbol{\phi}}_{\boldsymbol{n}v}, \hat{\boldsymbol{\phi}}_{\boldsymbol{n}'v'} \right\rangle_{L^2(\hat{K})^V} = \int_{\hat{K}} \left[\hat{\boldsymbol{\phi}}_{\boldsymbol{n}v}\right]_j \left[\hat{\boldsymbol{\phi}}_{\boldsymbol{n}'v'}\right]_j \, d\boldsymbol{\xi} = \\ &\left([\boldsymbol{e}_v]_j \, [\boldsymbol{e}_{v'}]_j\right) \int_0^1 \int_{\hat{K}} \hat{\phi}_{\boldsymbol{n}}\hat{\phi}_{\boldsymbol{n}'} \, d\boldsymbol{\xi} = \hat{\omega}_{\boldsymbol{n}}\delta_{\boldsymbol{n}\boldsymbol{n}'}\delta_{vv'} \end{aligned} \tag{2.56}$$

for all $\boldsymbol{n}, \boldsymbol{n}' \in \boldsymbol{\mathcal{N}}$ and $v, v' \in \{1, 2, \ldots, V\}$ the set is an orthogonal basis for $\mathbb{Q}_N(\hat{K})^V$.

Vector-valued basis functions on the space-time reference element

The set $\{\hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv}\}_{\boldsymbol{n}\in\boldsymbol{\mathcal{N}},l\in\mathcal{N},v\in\mathcal{V}}$ defined as

$$\hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv}(\boldsymbol{\xi}, \tau) = \hat{\theta}_{\boldsymbol{n}l}(\boldsymbol{\xi}, \tau)\boldsymbol{e}_v = \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi})\hat{\psi}_l(\tau)\boldsymbol{e}_v \tag{2.57}$$

is a basis of $\mathbb{Q}_N(\hat{K} \times [0, 1])^V$. Since furthermore

$$\left\langle \hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv}, \hat{\boldsymbol{\theta}}_{\boldsymbol{n}'l'v'} \right\rangle_{L^2\left(\hat{K}\times[0,1]\right)^V} = \int_0^1 \int_{\hat{K}} \left[\hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv}\right]_j \left[\hat{\boldsymbol{\theta}}_{\boldsymbol{n}'l'v'}\right]_j \, d\boldsymbol{\xi} \, d\tau = \hat{\omega}_{\boldsymbol{n}}\hat{\omega}_l\delta_{\boldsymbol{n}\boldsymbol{n}'}\delta_{ll'}\delta_{vv'}, \tag{2.58}$$

for all $\boldsymbol{n}, \boldsymbol{n}' \in \boldsymbol{\mathcal{N}}$, $l, l' \in \mathcal{N}$ and $v, v' \in \mathcal{V}$, the set is an orthogonal basis with respect to the respective L^2-scalar product.

2.1.9 Basis functions in global coordinates

We can use the mappings derived in ch. 2.1.7 to map the basis functions to global coordinates. For the vector-valued basis functions on a spatial element K we obtain

$$\boldsymbol{\phi}_{\boldsymbol{n}v}^K(\boldsymbol{x}) = \begin{cases} \left(\hat{\boldsymbol{\phi}}_{\boldsymbol{n}v} \circ \boldsymbol{\mathcal{X}}_K^{-1}\right)(\boldsymbol{x}) & \text{if } \boldsymbol{x} \in K \\ 0 & \text{otherwise,} \end{cases} \tag{2.59}$$

and for the vector-valued basis functions on a space-time element $K \times [t_i, t_i + \Delta t_i]$ we have

$$\boldsymbol{\theta}_{\boldsymbol{n}lv}^{Ki}(\boldsymbol{x}, t) = \begin{cases} \left(\hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv} \circ \left(\boldsymbol{\mathcal{X}}_K^{-1}, \mathcal{T}_i^{-1}\right)\right)(\boldsymbol{x}, t) & \text{if } \boldsymbol{x} \in K \text{ and } t \in [t_i, t_i + \Delta t_i] \\ 0 & \text{otherwise} \end{cases} \tag{2.60}$$

for $\boldsymbol{n} \in \boldsymbol{\mathcal{N}}$, $l \in \{0, 1, \ldots, N\}$ as well as $v \in \mathcal{V}$ and for all $K \in \mathcal{K}_h$ and $i \in \mathcal{I}$.

2.1.10 A fully-discrete iterative method for the space-time predictor

We recall relation (2.25) for the space-time predictor. Plugging in the initial condition (2.24) yields

$$\int_K \left[\left. \tilde{\boldsymbol{q}}_h^{K,i} \right|_{t_i+\Delta t_i} \right]_j \left[\left. \tilde{\boldsymbol{w}}_h^{K,i} \right|_{t_i+\Delta t_i} \right]_j d\boldsymbol{x} - \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\tilde{\boldsymbol{q}}_h^{K,i} \right]_j \frac{\partial}{\partial t} \left[\tilde{\boldsymbol{w}}_h^{K,i} \right]_j d\boldsymbol{x}\, dt =$$
$$\int_K \left[\left. \tilde{\boldsymbol{u}}_h^{K,i} \right|_{t_i} \right]_j \left[\left. \tilde{\boldsymbol{w}}_h^{K,i} \right|_{t_i} \right]_j d\boldsymbol{x} + \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{q}}_h^{K,i}) \right]_{jk} \frac{\partial}{\partial x_k} \left[\tilde{\boldsymbol{w}}_h^{K,i} \right]_j d\boldsymbol{x}\, dt +$$
$$\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{S}\left(\tilde{\boldsymbol{q}}_h^{K,i} \right) \right]_j \left[\tilde{\boldsymbol{w}}_h^{K,i} \right]_j d\boldsymbol{x}\, dt \tag{2.61}$$

which we require to hold for all $\tilde{\boldsymbol{w}}_h \in \tilde{\mathbb{W}}_h$, $K \in \mathcal{K}_h$ and $i \in \mathcal{I}$.

Making use of the bases we derived in the previous section the cell-local space-time predictor $\tilde{\boldsymbol{q}}_h^{K,i}$ can be represented by a tensor of coefficients $\hat{\boldsymbol{q}}^{K,i}$ ("degrees of freedom") as follows:

$$\tilde{\boldsymbol{q}}_h^{K,i} = \left[\hat{\boldsymbol{q}}^{K,i} \right]_{\boldsymbol{n}lv} \boldsymbol{\theta}_{\boldsymbol{n}lv}^{Ki}. \tag{2.62}$$

The initial condition $\left. \tilde{\boldsymbol{u}}_h^{K,i} \right|_{t_i}$ can be represented as

$$\left. \tilde{\boldsymbol{u}}_h^{K,i} \right|_{t_i} = \left[\hat{\boldsymbol{u}}^{K,i} \right]_{\boldsymbol{n}v} \boldsymbol{\phi}_{\boldsymbol{n}v}^{K}, \tag{2.63}$$

where

$$\left[\hat{\boldsymbol{u}}^{K,i} \right]_{\boldsymbol{n}v} = \left[\left. \tilde{\boldsymbol{u}}_h^{K,i} \right|_{\left(\boldsymbol{\mathcal{X}}_K(\boldsymbol{\xi_n}), t_i \right)} \right]_v. \tag{2.64}$$

Inserting eqs. (2.62) and (2.63) into eq. (2.61) and introduction of the iteration index $r \in \{0, 1, \ldots, R\}$ leads to the following iterative scheme for the degrees of freedom of the cell-local space-time predictor:

$$
\begin{aligned}
&\underbrace{\int_K \left[\left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{n}lv} \boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv}\Big|_{t_i+\Delta t_i} \right]_j \left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma}\Big|_{t_i+\Delta t_i} \right]_j d\boldsymbol{x}}_{\text{S-I}} - \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{n}lv} \boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv} \right]_j \frac{\partial}{\partial t} \left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma} \right]_j d\boldsymbol{x}\, dt}_{\text{S-II}} = \\
&\underbrace{\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n}v} \boldsymbol{\phi}^{K}_{\boldsymbol{n}v} \right]_j \left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma}\Big|_{t_i} \right]_j d\boldsymbol{x}}_{\text{S-III}} + \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv} \boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv} \right) \right]_{jk} \frac{\partial}{\partial x_k} \left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma} \right]_j d\boldsymbol{x}\, dt}_{\text{S-IV}} + \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv} \boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv} \right) \right]_{j} \left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma} \right]_j d\boldsymbol{x}\, dt}_{\text{S-V}} .
\end{aligned}
\tag{2.65}
$$

We require this relation to hold for all $\boldsymbol{\alpha} \in \boldsymbol{\mathcal{N}}$, $\beta \in \mathcal{N}$ and $\gamma \in \mathcal{V}$.

As initial condition, i.e. for $r = 0$, we use

$$
\left[\hat{\boldsymbol{q}}^{K,i,0}\right]_{\boldsymbol{n}vl} = \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n}v} \tag{2.66}
$$

for all time degrees of freedom $l \in \mathcal{N}$.

We will now proceed in a term-by-term fashion to rewrite all integrals with respect to reference coordinates so that we can finally derive a complete rule on how to compute $\hat{\boldsymbol{q}}^{K,i,r+1}$ that holds for all $K \in \mathcal{K}_h$.

Term S-I

The first term of eq. (2.65) can be rewritten with respect to reference coordinates as follows:

$$
\begin{aligned}
&\int_K \left[\left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{nlw} \boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv} \Big|_{t_i+\Delta t_i} \right]_j \left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma} \right]_{t_i+\Delta t_i} d\boldsymbol{x} = \\
&\int_K \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \phi^K_{\boldsymbol{n}} \left(\psi^i_l \Big|_{t_i+\Delta t_i} \right) [\boldsymbol{e}_v]_j \, \phi^K_{\boldsymbol{\alpha}} \left(\psi^i_\beta \Big|_{t_i+\Delta t_i} \right) \left[\boldsymbol{e}_\gamma \right]_j d\boldsymbol{x} = \\
&J_{\boldsymbol{x}_K} \int_{\hat{K}} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \hat{\phi}_{\boldsymbol{n}} \left(\hat{\psi}_l \Big|_1 \right) [\boldsymbol{e}_v]_j \, \hat{\phi}_{\boldsymbol{\alpha}} \left(\hat{\psi}_\beta \Big|_1 \right) \left[\boldsymbol{e}_\gamma \right]_j d\boldsymbol{\xi} = \\
&J_{\boldsymbol{x}_K} \sum_{\boldsymbol{\alpha}' \in \mathcal{N}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \hat{\phi}_{\boldsymbol{n}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \left(\hat{\psi}_l \Big|_1 \right) [\boldsymbol{e}_v]_j \, \hat{\phi}_{\boldsymbol{\alpha}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \left(\hat{\psi}_\beta \Big|_1 \right) \left[\boldsymbol{e}_\gamma \right]_j \right) = \\
&J_{\boldsymbol{x}_K} \sum_{\boldsymbol{\alpha}' \in \mathcal{N}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \delta_{\boldsymbol{n}\boldsymbol{\alpha}'} \left(\hat{\psi}_l \Big|_1 \right) \delta_{vj} \delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'} \left(\hat{\psi}_\beta \Big|_1 \right) \delta_{j\gamma} \right) = \\
&J_{\boldsymbol{x}_K} \hat{\omega}_{\boldsymbol{\alpha}} \underbrace{\left[\hat{\psi}_\beta \Big|_1 \hat{\psi}_l \Big|_1 \right]}_{[\text{FRm?}]_{\beta l}} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{\alpha}l\gamma},
\end{aligned}
\tag{2.67}
$$

where we remember from eq. (2.35) that

$$
J_{\boldsymbol{x}_K} = \prod_{d=1}^{D} [\Delta \boldsymbol{x}]_d \,. \tag{2.68}
$$

Term S-II

The second term of eq. (2.65) can be rewritten with respect to reference coordinates as follows:

$$
\begin{aligned}
&\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv} \right]_j \frac{\partial}{\partial t} \left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma} \right]_j \, d\boldsymbol{x}\, dt = \\
&\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \phi^K_{\boldsymbol{n}} \psi^i_l \left[\boldsymbol{e}_v \right]_j \phi^K_{\boldsymbol{\alpha}} \left(\frac{\partial}{\partial t} \psi^i_\beta \right) \left[\boldsymbol{e}_\gamma \right]_j \, d\boldsymbol{x}\, dt = \\
&J_{\mathcal{T}_i} J_{\boldsymbol{x}_K} \int_0^1 \int_{\hat{K}} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \hat{\phi}_{\boldsymbol{n}} \hat{\psi}_l \left[\boldsymbol{e}_v \right]_j \hat{\phi}_{\boldsymbol{\alpha}} \left(\frac{1}{\Delta t_i} \frac{\partial}{\partial \tau} \hat{\psi}_\beta \right) \left[\boldsymbol{e}_\gamma \right]_j \, d\boldsymbol{\xi}\, d\tau = \\
&J_{\mathcal{T}_i} J_{\boldsymbol{x}_K} \sum_{\boldsymbol{\alpha}' \in \boldsymbol{\mathcal{N}}} \sum_{\beta' \in \mathcal{N}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \hat{\omega}_{\beta'} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \hat{\phi}_{\boldsymbol{n}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \hat{\psi}_l(\hat{\tau}_{\beta'}) \left[\boldsymbol{e}_v \right]_j \dots \right. \\
&\qquad \left. \dots \hat{\phi}_{\boldsymbol{\alpha}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \left(\frac{\partial}{\partial \tau} \hat{\psi}_\beta(\hat{\tau}_{\beta'}) \right) \left[\boldsymbol{e}_\gamma \right]_j \right) = \\
&J_{\mathcal{T}_i} J_{\boldsymbol{x}_K} \sum_{\boldsymbol{\alpha}' \in \boldsymbol{\mathcal{N}}} \sum_{\beta' \in \mathcal{N}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \hat{\omega}_{\beta'} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \delta_{\boldsymbol{n}\boldsymbol{\alpha}'} \delta_{l\beta'} \delta_{vj} \dots \right. \\
&\qquad \left. \dots \delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'} \left(\frac{1}{\Delta t_i} \frac{\partial}{\partial \tau} \hat{\psi}_\beta(\hat{\tau}_{\beta'}) \right) \delta_{\gamma j} \right) = \\
&J_{\mathcal{T}_i} J_{\boldsymbol{x}_K} \hat{\omega}_{\boldsymbol{\alpha}} \frac{1}{\Delta t_i} \sum_{\beta' \in \mathcal{N}} \left(\underbrace{\hat{\omega}_{\beta'} \left[\frac{\partial}{\partial \tau} \hat{\psi}_\beta(\hat{\tau}_{\beta'}) \right]}_{\left[Kxi? \right]_{\beta\beta'}} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{\alpha}\beta'\gamma} \right),
\end{aligned}
\tag{2.69}
$$

where we remember from eq. (2.37) that

$$
J_{\mathcal{T}_i} = \Delta t_i, \tag{2.70}
$$

so that Δt_i and $1/\Delta t_i$ in eq. (2.69) cancel. In the derivation we made use of the fact that due to the chain rule

$$
\frac{\partial}{\partial t} \psi^i_\beta = \frac{\partial}{\partial t} \left(\hat{\psi}_\beta \circ \mathcal{T}_i^{-1} \right) = \left(\frac{\partial}{\partial \tau} \hat{\psi}_\beta \right) \left(\frac{\partial}{\partial t} \mathcal{T}_i^{-1} \right) = \frac{1}{\Delta t_i} \frac{\partial}{\partial \tau} \hat{\psi}_\beta. \tag{2.71}
$$

Term S-III

The third term of eq. (2.65) can be rewritten with respect to reference coordinates as follows:

$$
\begin{aligned}
&\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i}\right]_{nv} \boldsymbol{\phi}^K_{nv}\right]_j \left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma}\Big|_{t_i}\right]_j \, d\boldsymbol{x} = \\
&\int_K \left[\hat{\boldsymbol{u}}^{K,i}\right]_{nv} \phi^K_{\boldsymbol{n}} \left[\boldsymbol{e}_v\right]_j \phi^K_{\boldsymbol{\alpha}} \left(\psi^i_\beta\Big|_{t_i}\right) \left[\boldsymbol{e}_\gamma\right]_j \, d\boldsymbol{x} = \\
&J\boldsymbol{x}_K \int_{\hat{K}} \left[\hat{\boldsymbol{u}}^{K,i}\right]_{nv} \hat{\phi}_{\boldsymbol{n}} \left[\boldsymbol{e}_v\right]_j \hat{\phi}_{\boldsymbol{\alpha}} \left(\hat{\psi}_\beta\Big|_0\right) \left[\boldsymbol{e}_\gamma\right]_j \, d\boldsymbol{\xi} = \\
&J\boldsymbol{x}_K \sum_{\boldsymbol{\alpha}'\in\mathcal{N}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{u}}^{K,i}\right]_{nv} \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'}) \left[\boldsymbol{e}_v\right]_j \hat{\phi}_{\boldsymbol{\alpha}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'}) \left(\hat{\psi}_\beta\Big|_0\right) \left[\boldsymbol{e}_\gamma\right]_j\right) = \\
&J\boldsymbol{x}_K \sum_{\boldsymbol{\alpha}'\in\mathcal{N}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{u}}^{K,i}\right]_{nv} \delta_{\boldsymbol{n}\boldsymbol{\alpha}'}\delta_{vj}\delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'} \left(\hat{\psi}_\beta\Big|_0\right) \delta_{\gamma j}\right) = \\
&J\boldsymbol{x}_K \hat{\omega}_{\boldsymbol{\alpha}} \underbrace{\left[\hat{\psi}_\beta\Big|_0\right]}_{[\mathrm{F0}]_\beta} \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{\alpha}\gamma} .
\end{aligned}
\tag{2.72}
$$

Term S-IV

The third term of eq. (2.65) can be rewritten with respect to reference coordinates as follows:

$$
\begin{aligned}
&\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv} \boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv} \right)\right]_{jk} \frac{\partial}{\partial x_k} \left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma}\right]_j \, d\boldsymbol{x}\, dt = \\
&\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv} \phi^K_{\boldsymbol{n}} \psi^i_l \boldsymbol{e}_v \right)\right]_{jk} \left(\prod_{d=1,d\neq k}^{D} \psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d) \right) \psi^i_\beta(t) \left[\boldsymbol{e}_\gamma\right]_j \cdots \\
&\cdots \left(\frac{\partial}{\partial x_k} \psi^K_{[\boldsymbol{\alpha}]_k} \right) d\boldsymbol{x}\, dt = \\
&J_{\mathcal{T}_i} J_{\boldsymbol{x}_K} \int_0^1 \int_{\hat{K}} \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv} \hat{\phi}_{\boldsymbol{n}} \hat{\psi}_l \boldsymbol{e}_v \right)\right]_{jk} \left(\prod_{d=1,d\neq k}^{D} \hat{\psi}_{[\boldsymbol{\alpha}]_d}([\boldsymbol{\xi}]_d) \right) \hat{\psi}_\beta(t) \left[\boldsymbol{e}_\gamma\right]_j \cdots \\
&\cdots \left(\frac{1}{[\Delta \boldsymbol{x}]_k} \frac{\partial}{\partial \xi_k} \hat{\psi}_{[\boldsymbol{\alpha}]_k}([\boldsymbol{\xi}]_k) \right) d\boldsymbol{\xi}\, d\tau = \\
&J_{\mathcal{T}_i} J_{\boldsymbol{x}_K} \sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}} \sum_{\beta'\in\mathcal{N}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \hat{\omega}_{\beta'} \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv} \hat{\phi}_{\boldsymbol{n}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \hat{\psi}_l(\hat{\tau}_{\beta'}) \boldsymbol{e}_v \right)\right]_{jk} \cdots \right. \\
&\left. \cdots \left(\prod_{d=1,d\neq k}^{D} \hat{\psi}_{[\boldsymbol{\alpha}]_d} \left(\left[\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}\right]_d \right) \right) \hat{\psi}_\beta(\hat{\tau}_{\beta'}) \left[\boldsymbol{e}_\gamma\right]_j \left(\frac{1}{[\Delta \boldsymbol{x}]_k} \frac{\partial}{\partial \xi_k} \hat{\psi}_{[\boldsymbol{\alpha}]_k} \left(\left[\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}\right]_k \right) \right) \right) = \\
&J_{\mathcal{T}_i} J_{\boldsymbol{x}_K} \sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}} \sum_{\beta'\in\mathcal{N}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \hat{\omega}_{\beta'} \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv} \delta_{\boldsymbol{n}\boldsymbol{\alpha}'} \delta_{l\beta'} \boldsymbol{e}_v \right)\right]_{jk} \cdots \right. \\
&\left. \cdots \left(\prod_{d=1,d\neq k}^{D} \delta_{[\boldsymbol{\alpha}]_d [\boldsymbol{\alpha}']_d} \right) \delta_{\beta\beta'} \delta_{\gamma j} \left(\frac{1}{[\Delta \boldsymbol{x}]_k} \frac{\partial}{\partial \xi_k} \hat{\psi}_{[\boldsymbol{\alpha}]_k} \left(\left[\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}\right]_k \right) \right) \right) = \\
&J_{\mathcal{T}_i} J_{\boldsymbol{x}_K} \hat{\omega}_\beta \sum_{k=1}^{D} \left(\frac{1}{[\Delta \boldsymbol{x}]_k} \sum_{\alpha'_k \in \{0,1,\ldots,N\}} \left(\prod_{d=0,d\neq k}^{D} \hat{\omega}_{[\boldsymbol{\alpha}]_d} \cdots \right.\right. \\
&\left.\left. \cdots \underbrace{\hat{\omega}_{\alpha'_k} \left(\frac{\partial}{\partial \xi_k} \hat{\psi}_{[\boldsymbol{\alpha}]_k} \left(\hat{\xi}_{\alpha'_k} \right) \right)}_{[\mathrm{Kxi}]_{[\boldsymbol{\alpha}]_k \alpha'_k}} \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{[\alpha_0,\alpha_1,\ldots,\alpha_{k-1},\alpha'_k,\alpha_{k+1},\ldots,\alpha_N]\beta v} \boldsymbol{e}_v \right)\right]_{\gamma k} \right)\right),
\end{aligned}
\tag{2.73}
$$

where we used that

$$\frac{\partial}{\partial x_k}\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma}(\boldsymbol{x},t) = \left(\frac{\partial}{\partial x_k}\phi^K_{\boldsymbol{\alpha}}(\boldsymbol{x})\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma = \left(\frac{\partial}{\partial x_k}\prod_{d=1}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma =$$
$$\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\left(\frac{\partial}{\partial x_k}\psi^K_{[\boldsymbol{\alpha}]_k}([\boldsymbol{x}]_k)\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma =$$
$$\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\left(\frac{\partial}{\partial x_k}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x})\right]_k\right)\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma =$$
$$\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\left(\left(\frac{\partial}{\partial \xi_k}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x})\right]_k\right)\right)\left(\frac{\partial}{\partial x_k}\left[\boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x})\right]_k\right)\right)\dots$$
$$\dots\psi^i_\beta(t)\boldsymbol{e}_\gamma =$$
$$\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\left(\frac{1}{\left[\Delta\boldsymbol{x}^K\right]_k}\frac{\partial}{\partial \xi_k}\hat{\phi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x})\right]_k\right)\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma. \tag{2.74}$$

Term S-V

The fifth term of eq. (2.65) can be rewritten with respect to reference coordinates as follows:

$$\int_{t_i}^{t_i+\Delta t_i}\int_K\left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv}\boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv}\right)\right]_j\left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma}\right]_j d\boldsymbol{x}\,dt =$$
$$J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\int_0^1\int_{\hat{K}}\left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv}\hat{\phi}_{\boldsymbol{n}}\hat{\psi}_l\boldsymbol{e}_v\right)\right]_j\hat{\phi}_{\boldsymbol{\alpha}}\hat{\psi}_l\left[\boldsymbol{e}_\gamma\right]_j d\boldsymbol{\xi}\,d\tau =$$
$$J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}}\sum_{\beta'\in\mathcal{N}}\left(\hat{\omega}_{\boldsymbol{\alpha}'}\hat{\omega}_{\beta'}\left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv}\hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'})\hat{\psi}_l(\hat{\tau}_{\beta'})\boldsymbol{e}_v\right)\right]_j\dots\right.$$
$$\left.\dots\hat{\phi}_{\boldsymbol{\alpha}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'})\hat{\psi}_\beta(\hat{\tau}_{\beta'})\left[\boldsymbol{e}_\gamma\right]_j\right) = \tag{2.75}$$
$$J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}}\sum_{\beta'\in\mathcal{N}}\left(\hat{\omega}_{\boldsymbol{\alpha}'}\hat{\omega}_{\beta'}\left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv}\delta_{\boldsymbol{n}\boldsymbol{\alpha}'}\delta_{l\beta'}\boldsymbol{e}_v\right)\right]_j\delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'}\delta_{\beta\beta'}\delta_{\gamma j}\right) =$$
$$J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\hat{\omega}_{\boldsymbol{\alpha}}\hat{\omega}_\beta\left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{\alpha}\beta v}\boldsymbol{e}_v\right)\right]_\gamma$$

The complete fixed-point iteration for the space-time predictor

Now collecting the results from eqs. (2.67), (2.69), (2.72), (2.73) and (2.75) and plugging them back into eq. (2.65) and division by $J_{\mathcal{X}_K}$ yields TODO: division by omega alpha

$$
\begin{aligned}
&\hat{\omega}_{\boldsymbol{\alpha}} [\mathbf{FRm}]_{\beta\beta'} \left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{\alpha}\beta'\gamma} - \\
&\hat{\omega}_{\boldsymbol{\alpha}} [\mathbf{Kxi}]_{\beta\beta'} \left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{\alpha}\beta'\gamma} = \\
&\hat{\omega}_{\boldsymbol{\alpha}} \underbrace{\left[\hat{\psi}_\beta\Big|_0\right]}_{[\mathrm{F0}]_\beta} \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{\alpha}\gamma} + \\
&J_{\mathcal{T}_i}\hat{\omega}_\beta \sum_{k=1}^{D} \left(\frac{1}{[\Delta \boldsymbol{x}]_k} \sum_{\alpha'_k \in \{0,1,\dots,N\}} \left(\prod_{d=0, d\neq k}^{D} \hat{\omega}_{[\boldsymbol{\alpha}]_d} \cdots \right.\right. \\
&\left.\left. \dots [\mathbf{Kxi}]_{[\boldsymbol{\alpha}]_k \alpha'_k} \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{[\alpha_0,\alpha_1,\dots,\alpha_{k-1},\alpha'_k,\alpha_{k+1},\dots,\alpha_N]\beta v} \boldsymbol{e}_v \right)\right]_{\gamma k} \right)\right) + \\
&J_{\mathcal{T}_i}\hat{\omega}_{\boldsymbol{\alpha}}\hat{\omega}_\beta \left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{\alpha}\beta v} \boldsymbol{e}_v \right)\right]_\gamma ,
\end{aligned}
\tag{2.76}
$$

which has to hold for all $\boldsymbol{\alpha} \in \boldsymbol{\mathcal{N}}$, $\beta \in \mathcal{N}$ and $\gamma \in \mathcal{V}$.

Next step: $[\mathbf{K1}] = [\mathbf{FRm}] - [\mathbf{Kxi}]$. Precompute $[\mathbf{iK1}] = \left([\mathbf{FRm}] - [\mathbf{Kxi}]\right)^{-1}$ in advance.

TODO: Add appendix with code that computes all matrices

2.1.11 A fully discrete update scheme for the time-discrete solution

Now that we have developed a method to compute the space-time predictor, we can go back to the original one-step, cell-local update scheme given in eq. (2.21). Inserting the local space-time predictor $\tilde{\boldsymbol{q}}_h^{K,i}$ yields

$$
\begin{aligned}
&\int_K \left[\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i+\Delta t_i} \right]_v \left[\boldsymbol{w}_h^K\right]_v d\boldsymbol{x} = \int_K \left[\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i} \right]_v \left[\boldsymbol{w}_h^K\right]_v d\boldsymbol{x} + \\
&\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{q}}_h^{K,i})\right]_{vd} \frac{\partial}{\partial x_d} \left[\boldsymbol{w}_h^K\right]_v d\boldsymbol{x}\, dt + \\
&\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{S}\left(\hat{\boldsymbol{q}}^{K,i}\right)\right]_v \left[\boldsymbol{w}_h^K\right]_v d\boldsymbol{x}\, dt - \\
&\int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{\mathcal{G}}\left(\tilde{\boldsymbol{q}}_h^{K,i}, \tilde{\boldsymbol{q}}_h^{K^+ i}, \boldsymbol{n}\right)\right]_v \left[\boldsymbol{w}_h^K\right]_v ds(\boldsymbol{x})\, dt,
\end{aligned}
\tag{2.77}
$$

which has to hold for all $v \in \mathcal{V}$, $K \in \mathcal{K}_h$, $\boldsymbol{w}_h \in \mathbb{W}_h$ and $i \in \mathcal{I}$.

Making use of the bases we derived earlier the call-local solution $\tilde{\boldsymbol{u}}_h^{K,i}$ at times $t = t_i$ and $t = t_i + \Delta t_i$ can be represented by tensors of coefficients $\hat{\boldsymbol{u}}^{K,i}$ and $\hat{\boldsymbol{u}}^{K,i+1}$ as

$$\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i} = \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n},v} \boldsymbol{\phi}_{\boldsymbol{n},v}^K \tag{2.78}$$

and

$$\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i+\Delta t_i} = \left[\hat{\boldsymbol{u}}^{K,i+1}\right]_{\boldsymbol{n},v} \boldsymbol{\phi}_{\boldsymbol{n},v}^K, \tag{2.79}$$

respectively. Inserting eqs. (2.78) and (2.79) and the ansatz for the space-time predictor (2.62) into eq. (2.77) yields

$$\begin{aligned}
&\underbrace{\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i+1}\right]_{\boldsymbol{n},v} \boldsymbol{\phi}_{\boldsymbol{n},v}^K\right]_j \left[\boldsymbol{\phi}_{\boldsymbol{\alpha},\gamma}^K\right]_j d\boldsymbol{x}}_{\text{U-I}} = \underbrace{\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n},v} \boldsymbol{\phi}_{\boldsymbol{n},v}^K\right]_j \left[\boldsymbol{\phi}_{\boldsymbol{\alpha},\gamma}^K\right]_j}_{\text{U-II}} + \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v} \boldsymbol{\theta}_{\boldsymbol{n},l,v}^{Ki}\right)\right]_{jk} \frac{\partial}{\partial x_k} \left[\boldsymbol{\phi}_{\boldsymbol{\alpha},\gamma}^K\right]_j d\boldsymbol{x}\, dt}_{\text{U-III}} + \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v} \boldsymbol{\theta}_{\boldsymbol{n},l,v}^{Ki}\right)\right]_j \left[\boldsymbol{\phi}_{\boldsymbol{\alpha},\gamma}^K\right]_j d\boldsymbol{x}\, dt}_{\text{U-IV}} - \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{\mathcal{G}}\left(\hat{\boldsymbol{q}}^{K,i}, \hat{\boldsymbol{q}}^{K^+,i}, \boldsymbol{n}\right)\right]_j \left[\boldsymbol{\phi}_{\boldsymbol{\alpha},\gamma}^K\right]_j ds(\boldsymbol{x})\, dt}_{\text{U-V}},
\end{aligned} \tag{2.80}$$

which we require to hold for all $\boldsymbol{\alpha} \in \boldsymbol{\mathcal{N}}$, $\gamma \in \mathcal{V}$, $K \in \mathcal{K}_h$ and $i \in \mathcal{I}$. In the following we will again proceed by simplifying each term in reference coordinates separately and then in the end assemble all terms to obtain a complete fully-discrete update scheme.

Term U-I

The first term of eq. (2.80) can be rewritten with respect to reference coordinates as follows:

$$\begin{aligned}
&\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i+1}\right]_{\boldsymbol{n},v} \boldsymbol{\phi}^K_{\boldsymbol{n},v}\right]_j \left[\boldsymbol{\phi}^K_{\boldsymbol{\alpha},\gamma}\right]_j \, d\boldsymbol{x} = \\
&\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i+1}\right]_{\boldsymbol{n},v} \phi^K_{\boldsymbol{n}} \boldsymbol{e}_v\right]_j \left[\phi^K_{\boldsymbol{\alpha}} \boldsymbol{e}_\gamma\right]_j \, d\boldsymbol{x} = \\
&J_{\boldsymbol{\chi}_K} \int_{\hat{K}} \left[\left[\hat{\boldsymbol{u}}^{K,i+1}\right]_{\boldsymbol{n},v} \hat{\phi}_{\boldsymbol{n}} \boldsymbol{e}_v\right]_j \left[\hat{\phi}_{\boldsymbol{\alpha}} \boldsymbol{e}_\gamma\right]_j \, d\boldsymbol{\xi} = \\
&J_{\boldsymbol{\chi}_K} \sum_{\boldsymbol{\alpha}' \in \boldsymbol{\mathcal{N}}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{u}}^{K,i+1}\right]_{\boldsymbol{n},v} \hat{\phi}_{\boldsymbol{n}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \left[\boldsymbol{e}_v\right]_j \hat{\phi}_{\boldsymbol{\alpha}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \left[\boldsymbol{e}_\gamma\right]_j\right) = \\
&J_{\boldsymbol{\chi}_K} \sum_{\boldsymbol{\alpha}' \in \boldsymbol{\mathcal{N}}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{u}}^{K,i+1}\right]_{\boldsymbol{n},v} \delta_{\boldsymbol{n}\boldsymbol{\alpha}'} \delta_{vj} \delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'} \delta_{\gamma j}\right) = \\
&J_{\boldsymbol{\chi}_K} \hat{\omega}_{\boldsymbol{\alpha}} \left[\hat{\boldsymbol{u}}^{K,i+1}\right]_{\boldsymbol{\alpha},\gamma} .
\end{aligned} \tag{2.81}$$

Term U-II

Analogously to the first term of eq. (2.80), the second term can be rewritten as follows:

$$\begin{aligned}
&\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n},v} \boldsymbol{\phi}^K_{\boldsymbol{n},v}\right]_j \left[\boldsymbol{\phi}^K_{\boldsymbol{\alpha},\gamma}\right]_j \, d\boldsymbol{x} = \\
&J_{\boldsymbol{\chi}_K} \hat{\omega}_{\boldsymbol{\alpha}} \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{\alpha},\gamma} .
\end{aligned} \tag{2.82}$$

Term U-III

The third term of eq. (2.80) can be rewritten with respect to reference coordinates as follows:

$$
\begin{aligned}
&\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v} \boldsymbol{\theta}^{Ki}_{\boldsymbol{n},l,v} \right)\right]_{jk} \frac{\partial}{\partial x_k} \left[\boldsymbol{\phi}^K_{\boldsymbol{\alpha},\gamma}\right]_j \, d\boldsymbol{x}\, dt = \\
&\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v} \phi^K_{\boldsymbol{n}} \psi^i_l \boldsymbol{e}_v \right)\right]_{jk} \frac{\partial}{\partial x_k} \left(\prod_{d=1}^{D} \psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d) \right) \left[\boldsymbol{e}_\gamma\right]_j \, d\boldsymbol{x}\, dt = \\
&\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},v,l} \phi^K_{\boldsymbol{n}} \psi^i_l \boldsymbol{e}_v \right)\right]_{jk} \left(\prod_{d=1,d\neq k}^{D} \psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d) \right) \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_k} \frac{\partial}{\partial \xi_k} \hat{\psi}_{[\boldsymbol{\alpha}]_k} \left(\left[\boldsymbol{\mathcal{X}}_K(\boldsymbol{x})\right]_k \right) \left[\boldsymbol{e}_\gamma\right]_j \, d\boldsymbol{x} \\
&J_{\mathcal{T}_i} J_{\boldsymbol{\mathcal{X}}_K} \int_0^1 \int_{\hat{K}} \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v} \hat{\phi}_{\boldsymbol{n}} \hat{\psi}_l \boldsymbol{e}_v \right)\right]_{kj} \left(\prod_{d=1,d\neq k}^{D} \hat{\psi}[\boldsymbol{\alpha}]_d([\boldsymbol{\xi}]_d) \right) \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_k} \frac{\partial}{\partial \xi_k} \hat{\psi}_{[\boldsymbol{\alpha}]_k} \left([\boldsymbol{\xi}]_k \right) \left[\boldsymbol{e}_\gamma\right]_j \, d\boldsymbol{\xi}\, d\tau \\
&J_{\mathcal{T}_i} J_{\boldsymbol{\mathcal{X}}_K} \sum_{\boldsymbol{\alpha}' \in \boldsymbol{\mathcal{N}}} \sum_{\beta' \in \mathcal{N}} \Bigg(\hat{\omega}_{\boldsymbol{\alpha}'} \hat{\omega}_{\beta'} \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v} \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'}) \hat{\psi}(\hat{\tau}_{\beta'}) \boldsymbol{e}_v \right)\right]_{jk} \left(\prod_{d=1,d\neq k}^{D} \hat{\psi}_{[\boldsymbol{\alpha}]_d}([\boldsymbol{\xi}_{\boldsymbol{\alpha}'}]_d) \right) \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_k} \frac{\partial}{\partial \xi_k} \hat{\psi} \\
&J_{\mathcal{T}_i} J_{\boldsymbol{\mathcal{X}}_K} \sum_{\boldsymbol{\alpha}' \in \boldsymbol{\mathcal{N}}} \sum_{\beta' \in \mathcal{N}} \Bigg(\hat{\omega}_{\boldsymbol{\alpha}'} \hat{\omega}_{\beta'} \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v} \delta_{\boldsymbol{n}\boldsymbol{\alpha}'} \delta_{l\beta'} \boldsymbol{e}_v \right)\right]_{jk} \left(\prod_{d=1,d\neq k}^{D} \delta_{[\boldsymbol{\alpha}]_d [\boldsymbol{\alpha}']_d} \right) \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_k} \frac{\partial}{\partial \xi_k} \hat{\psi}_{[\boldsymbol{\alpha}]_k} \left([\boldsymbol{\xi}_{\boldsymbol{\alpha}'}]_k \right) \\
&J_{\mathcal{T}_i} J_{\boldsymbol{\mathcal{X}}_K} \hat{\omega}_{\boldsymbol{\alpha}} \sum_{k=1}^{D} \Bigg(\sum_{\alpha'_k \in \mathcal{N}} \sum_{\beta' \in \mathcal{N}} \Bigg(\frac{\hat{\omega}_{\beta'}}{\hat{\omega}_{\alpha'_k}} \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_k} \underbrace{\frac{\partial}{\partial \xi_k} \hat{\psi}_{\alpha'_k} \left(\left[\hat{\boldsymbol{\xi}}\right]_{\alpha'_k} \right)}_{\mathrm{Kxi}_{\alpha'_k k}} \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{[[\boldsymbol{\alpha}]_1,[\boldsymbol{\alpha}]_2,\ldots,[\boldsymbol{\alpha}]_{k-1},\alpha'_k,[\boldsymbol{\alpha}]_{k+1},\ldots,[\boldsymbol{\alpha}]_D],\beta',v} \right.\right.
\end{aligned}
\tag{2.83}
$$

where we made use of the fact that du to the chain rule:

$$
\begin{aligned}
&\frac{\partial}{\partial x_k}\left(\prod_{d=1}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right) = \left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\frac{\partial}{\partial x_k}\psi^K_{[\boldsymbol{\alpha}]_k}([\boldsymbol{x}]_k) = \\
&\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\frac{\partial}{\partial\xi_j}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}_K(\boldsymbol{x})\right]_k\right)\frac{\partial}{\partial x_k}\left[\boldsymbol{\mathcal{X}}_K(\boldsymbol{x})\right]_j = \\
&\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\frac{\partial}{\partial\xi_j}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}_K(\boldsymbol{x})\right]_k\right)\frac{1}{\left[\Delta\boldsymbol{x}^K\right]_k}\delta_k j = \\
&\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\frac{1}{\left[\Delta\boldsymbol{x}^K\right]_k}\frac{\partial}{\partial\xi_k}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}_K(\boldsymbol{x})\right]_k\right)\,d\boldsymbol{x}\,dt.
\end{aligned}
\tag{2.84}
$$

Term U-IV

The fourth term of eq. (2.80) can be rewritten with respect to reference coordinates as follows:

$$
\begin{aligned}
&\int_{t_i}^{t_i+\Delta t_i}\int_K\left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v}\boldsymbol{\theta}^{Ki}_{\boldsymbol{n},l,v}\right)\right]_j\left[\boldsymbol{\phi}^K_{\boldsymbol{\alpha},\gamma}\right]_j\,d\boldsymbol{x}\,dt = \\
&\int_{t_i}^{t_i+\Delta t_i}\int_K\left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v}\phi^K_{\boldsymbol{n}}\psi^i_l\boldsymbol{e}_v\right)\right]_j\phi^K_{\boldsymbol{\alpha}}\left[\boldsymbol{e}_\gamma\right]_j\,d\boldsymbol{x}\,dt = \\
&J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\int_0^1\int_{\hat{K}}\left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v}\hat{\phi}_{\boldsymbol{n}}\hat{\psi}_l\boldsymbol{e}_v\right)\right]_j\hat{\phi}_{\boldsymbol{\alpha}}\left[\boldsymbol{e}_\gamma\right]_j\,d\boldsymbol{\xi}\,d\tau = \\
&J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}}\sum_{\beta'\in\mathcal{N}}\left(\hat{\omega}_{\boldsymbol{\alpha}'}\hat{\omega}_{\beta'}\left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v}\hat{\phi}_{\boldsymbol{n}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'})\hat{\psi}_l(\hat{\tau}_{\beta'}\boldsymbol{e}_v)\right)\right]_j\hat{\phi}_{\boldsymbol{\alpha}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'})\left[\boldsymbol{e}_\gamma\right]_j\right) = \\
&J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}}\sum_{\beta'\in\mathcal{N}}\left(\hat{\omega}_{\boldsymbol{\alpha}'}\hat{\omega}_{\beta'}\left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v}\delta_{\boldsymbol{n}\boldsymbol{\alpha}'}\delta_{l\beta'}\boldsymbol{e}_v)\right)\right]_j\delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'}\delta_{\gamma j}\right) = \\
&J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\hat{\omega}_{\boldsymbol{\alpha}}\sum_{\beta'\in\mathcal{N}}\left(\hat{\omega}_{\beta'}\left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{\alpha},\beta',v}\boldsymbol{e}_v\right)\right]_\gamma\right).
\end{aligned}
\tag{2.85}
$$

Term U-V

Let $d \in \mathcal{D}$ and $e \in \{0,1\} := \mathcal{E}$. Then if we define the $D-1$-dimensional quadrilateral $\partial\hat{K}_{d,e}$ as

$$
\partial\hat{K}_{d,e} = \left\{\boldsymbol{\xi}\in\hat{K} \mid \left[\boldsymbol{\xi}\right]_d = e\right\},
\tag{2.86}
$$

the set $\{\partial\hat{K}_{d,e}\}_{d\in\mathcal{D},e\in\mathcal{E}}$ is a partition of the surface $\partial\hat{K}$ of the spatial reference element. By making use of the mappings $\boldsymbol{\mathcal{X}}_K$ that maps points $\boldsymbol{\xi} \in \hat{K}$ to $\boldsymbol{x} \in K$ for all $K \in \mathcal{K}_h$ we can define

$$\partial K_{d,e} = \boldsymbol{\mathcal{X}}_K \left(\partial\hat{K}_{d,e}\right), \tag{2.87}$$

where now the set $\{\partial K_{d,e}\}_{d\in\mathcal{D},e\in\mathcal{E}}$ is a quadrilateral partition of the surface ∂K for all cells $K \in \mathcal{K}_h$.

In consequence the surface integral in the fifth term of eq. (2.80) can be rewritten as follows:

$$\begin{aligned}
&\int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{\mathcal{G}}\left(\hat{\boldsymbol{q}}^{K,i}, \hat{\boldsymbol{q}}^{K^+,i}, \boldsymbol{n}\right)\right]_j \left[\boldsymbol{\phi}^K_{\boldsymbol{\alpha},\gamma}\right]_j ds(\boldsymbol{x})\, dt = \\
&\int_{t_i}^{t_i+\Delta t_i} \sum_{d\in\mathcal{D}} \sum_{e\in\mathcal{E}} \left(\int_{\partial K_{d,e}} \left[\boldsymbol{\mathcal{G}}\left(\hat{\boldsymbol{q}}^{K,i}, \hat{\boldsymbol{q}}^{K^+,i}, \boldsymbol{e}_d\right)\right]_j \phi^K_{\boldsymbol{\alpha}} \left[\boldsymbol{e}_\gamma\right]_j ds(\boldsymbol{x}) \right) dt = \\
&J_{\mathcal{T}_i} J_{\boldsymbol{\mathcal{X}}_K} \int_0^1 \sum_{d\in\mathcal{D}} \sum_{e\in\mathcal{E}} \left(\frac{1}{\left[\Delta \boldsymbol{x}^K\right]_d} \int_{\partial\hat{K}_{d,e}} \left[\boldsymbol{\mathcal{G}}\left(\hat{\boldsymbol{q}}^{K,i}, \hat{\boldsymbol{q}}^{K^+,i}, (-1)^e \boldsymbol{e}_d\right)\right]_j \hat{\phi}_{\boldsymbol{\alpha}} \left[\boldsymbol{e}_d\right]_j ds(\boldsymbol{\xi}) \right) d\tau = \\
&J_{\mathcal{T}_i} J_{\boldsymbol{\mathcal{X}}_K} \sum_{\beta'\in\mathcal{D}} \hat{\omega}_{\beta'} \sum_{d\in\mathcal{D}} \sum_{e\in\mathcal{E}} \sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}^-} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_d} \left[\boldsymbol{\mathcal{G}}\left(\hat{\boldsymbol{q}}^{K,i}, \hat{\boldsymbol{q}}^{K^+,i}, (-1)^e \boldsymbol{e}_d\right)\right]_j \hat{\phi}_{\boldsymbol{\alpha}^d}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \left(\hat{\psi}_{[\boldsymbol{\alpha}]_d}\Big|_e \right) \left[\boldsymbol{e}_d\right]_j \right) = \\
&J_{\mathcal{T}_i} J_{\boldsymbol{\mathcal{X}}_K} \sum_{\beta'\in\mathcal{D}} \hat{\omega}_{\beta'} \sum_{d\in\mathcal{D}} \sum_{e\in\mathcal{E}} \sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}^-} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_d} \left[\boldsymbol{\mathcal{G}}\left(\hat{\boldsymbol{q}}^{K,i}, \hat{\boldsymbol{q}}^{K^+,i}, (-1)^e \boldsymbol{e}_d\right)\right]_j \delta_{\boldsymbol{\alpha}^d \boldsymbol{\alpha}'} \left(\hat{\psi}_{[\boldsymbol{\alpha}]_d}\Big|_e \right) \delta_{\gamma j} \right) = \\
&J_{\mathcal{T}_i} J_{\boldsymbol{\mathcal{X}}_K} \hat{\omega}_{\boldsymbol{\alpha}} \sum_{\beta'\in\mathcal{D}} \sum_{d\in\mathcal{D}} \sum_{e\in\mathcal{E}} \sum_{\alpha'_d\in\mathcal{N}} \left(\frac{\hat{\omega}_{\beta'}}{\hat{\omega}_{\alpha'_d}} \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_d} \left[\boldsymbol{\mathcal{G}}\left(\hat{\boldsymbol{q}}^{K,i}, \hat{\boldsymbol{q}}^{K^+,i}, (-1)^e \boldsymbol{e}_d\right)\right]_\gamma \underbrace{\left(\hat{\psi}_{\alpha'_d}\Big|_e \right)}_{\text{F0, F1}} \right).
\end{aligned} \tag{2.88}$$

In each term we have to solve a Riemann problem in direction of the unit vector $\boldsymbol{e}_d$ defined as

$$\left[\boldsymbol{e}_d\right]_{d'} = \delta_{dd'} \tag{2.89}$$

for $d' \in \mathcal{D}$.

The complete one-step update formula

Inserting eqs. (2.81) to (2.83), (2.85) and (2.88) into eq. (2.80) and dividing the resulting equation by $\hat{\omega}_{\boldsymbol{\alpha}}$ and $J_{\boldsymbol{\mathcal{X}}_K}$ yields

$$\begin{aligned}
&\left[\hat{\boldsymbol{u}}^{K,i+1}\right]_{\boldsymbol{\alpha},\gamma} = \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{\alpha},\gamma} + \\
&J_{\mathcal{T}_i} \sum_{k=1}^{D} \left(\sum_{\alpha'_k \in \mathcal{N}} \sum_{\beta' \in \mathcal{N}} \left(\frac{\hat{\omega}_{\beta'}}{\hat{\omega}_{\alpha'_k}} \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_k} \underbrace{\frac{\partial}{\partial \xi_k} \hat{\psi}_{\alpha'_k}\left(\left[\hat{\boldsymbol{\xi}}\right]_{\alpha'_k}\right)}_{\mathrm{Kxi}_{\alpha'_k k}} \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\left[[\boldsymbol{\alpha}]_1,[\boldsymbol{\alpha}]_2,\ldots,[\boldsymbol{\alpha}]_{k-1},\alpha'_k,[\boldsymbol{\alpha}]_{k+1},\ldots,[\boldsymbol{\alpha}]_D\right],\beta',v} \boldsymbol{e}_v \right) \right]_{\gamma,k} \right) \right) + \\
&J_{\mathcal{T}_i} \sum_{\beta' \in \mathcal{N}} \left(\hat{\omega}_{\beta'} \left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{\alpha},\beta',v} \boldsymbol{e}_v \right) \right]_{\gamma} \right) - \\
&J_{\mathcal{T}_i} \sum_{\beta' \in \mathcal{D}} \sum_{d \in \mathcal{D}} \sum_{e \in \mathcal{E}} \sum_{\alpha'_d \in \mathcal{N}} \left(\frac{\hat{\omega}_{\beta'}}{\hat{\omega}_{\alpha'_d}} \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_d} \left[\boldsymbol{\mathcal{G}}\left(\hat{\boldsymbol{q}}^{K,i}, \hat{\boldsymbol{q}}^{K^+,i}, (-1)^e \boldsymbol{e}_d \right) \right]_{\gamma} \underbrace{\left(\hat{\psi}_{\alpha'_d}\Big|_e \right)}_{\mathrm{F0,\ F1}} \right),
\end{aligned} \tag{2.90}$$

which we require to hold for $\boldsymbol{\alpha} \in \boldsymbol{\mathcal{N}}$, $\gamma \in \mathcal{V}$, $K \in \mathcal{K}_h$ and $i \in \mathcal{I}$.

Time step restriction

$$\Delta t \leq \frac{1}{D} \frac{1}{(2N+1)} \min_{d \in \mathcal{D}} \left(\frac{[\Delta \boldsymbol{x}]_d}{\Lambda^d} \right), \tag{2.91}$$

where

$$\Lambda^d = \underset{v \in \mathcal{V}}{\mathrm{maxabs}} \left[\boldsymbol{\lambda}^d \right]_v \tag{2.92}$$

and $\boldsymbol{\lambda}^d$ is a vector containing the V real eigenvalues of the Jacobian

$$\frac{\partial}{\partial x_j} \left[\boldsymbol{F}\left(\boldsymbol{u}(\boldsymbol{x},t) \right) \right]_{id} \tag{2.93}$$

for the respective dimension $d \in \mathcal{D}$.

2.1.12 A posteriori subcell limiting

Motivation:

- Shock = discontinuity

- Discontinuity + high-order DG method leads to Gibbs phenomenon (oscillations)
- Reason: Discon. initial data or spontaneous formation in nonlinear problems
- Problems:
    1. Pointwise first order away from discontinuity
    2. Loss of pointwise convergence at the point of discontinuity
    3. Introduction of artificial and persistent oscillations at the point of discontinuity
- Positive physical quantities such as pressure or density might become negative; simulation might crash
- ADER-DG with a posteriori subcell limiting has very desirable properties (TODO)

Questions:

1. How do we identify cells for which limiting is needed? Troubled cell indicator.
2. How do we achieve high-order accuracy and still ensure non-oscillatory property close to troubled cells? Ideally replace DG solution such that additional numerical viscosity is added only at these cells but nowhere else and preferably without destroying the subcell resolution of the DG method.

Projection and reconstruction

In order to do FVM we need to project the ADER-DG degrees of freedom $\hat{\boldsymbol{u}}^{K,i}$ to N_S equidistant subcell-averages $\hat{\boldsymbol{p}}^{K_L,i}$ for each cell $K \in \mathcal{K}_h$. We choose $N_S = 2N + 1$, since for explicit Godunov-type finite volume schemes on the subgrid we must satisfy the stability condition

$$\Delta t \leq \frac{1}{d} \frac{1}{N_S} \min_{d \in \mathcal{D}} \left(\frac{[\Delta \boldsymbol{x}]_d}{\Lambda^d} \right). \tag{2.94}$$

Comparing eq. (2.94) to the time step restriction for the ADER-DG scheme given in eq. (2.91) illustrates that the choice $N_S = 2N + 1$ make sure that a) time steps on the ADER-DG grid are also valid on the subgrid and b) that we add the minimum amount of dissipation.

Let L^K be a regular subgrid on cell K consisting of $(N_s)^D = (2N+1)^D$ subcells denoted by $L_{\boldsymbol{j}}^K$, $\boldsymbol{j} \in \{1, 2, \ldots, (N_S)^D\} := \boldsymbol{\mathcal{N}_S}$ for $N_S \geq N + 1$. Then we can define an alternative representation of the $V(N+1)^D$ degrees of freedom $\hat{\boldsymbol{u}}^{K,i}$ in terms of $V(N_S)^D$ cell averages $\hat{\boldsymbol{p}}^{K_L,i}$ using the following relation:

$$\begin{aligned}
\left[\hat{\boldsymbol{p}}^{K_L,i}\right]_{\boldsymbol{\alpha},\gamma} =& \frac{1}{|L_K^{\boldsymbol{\alpha}}|}\int_{L_K^{\boldsymbol{\alpha}}} \left[\tilde{\boldsymbol{u}}_h^{K,i}\right]_\gamma \, d\boldsymbol{x} = \frac{1}{|L_K^{\boldsymbol{\alpha}}|}\int_{L_K^{\boldsymbol{\alpha}}} \phi_{\boldsymbol{n}}^K(\boldsymbol{x}) \left[\boldsymbol{e}_v\right]_\gamma \, d\boldsymbol{x} \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n},v} = \\
& \int_{\hat{K}} \hat{\phi}_{\boldsymbol{n}}\left(\frac{1}{N_S}\boldsymbol{\alpha} + \frac{1}{N_S}\boldsymbol{\xi}\right) d\xi \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n},\gamma} = \\
& \sum_{\alpha' \in \boldsymbol{\mathcal{N}}} \left(\hat{\omega}_{\boldsymbol{\alpha}'}\hat{\phi}_{\boldsymbol{n}}\left(\frac{1}{N_S}\boldsymbol{\alpha} + \frac{1}{N_S}\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}\right)\right) \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n},\gamma} = \\
& a
\end{aligned} \tag{2.95}$$

We can directly derive the following relation:

Reconstruction: If $N_S > N+1$ then we impose additional restrictions:

Identification of troubled cells

Candidate solution: $\boldsymbol{u}_h^*(\boldsymbol{x}, t^{i+1})$ obtained using unlimited high-order scheme. Apply troubled cell indicator Project, recompute with more robust scheme and restrict.

Physical admissibility detection (PAD): Domain knowledge

$$\pi_k\left(\boldsymbol{u}_h^*(\boldsymbol{x}, t^{i+1})\right) > 0 \tag{2.96}$$

For Euler $\pi_1(\boldsymbol{u}) = \rho$, $\pi_2(\boldsymbol{u}) = p$.

Numerical admissibility detection (NAD): Relaxed discrete maximum principle:

$$\min_{\boldsymbol{x}' \in V(K)} \boldsymbol{u}_h(\boldsymbol{x}', t^i) - \delta \leq \boldsymbol{u}_h^*(\boldsymbol{x}, t^{i+1}) \leq \min_{\boldsymbol{x}' \in V(K)} \boldsymbol{u}_h(\boldsymbol{x}', t^i) + \delta \tag{2.97}$$

for all Voronoi neighbors K' of $K \in \mathcal{K}_h$.

Proposed relaxation:

$$\delta = \varepsilon\left(\max_{\boldsymbol{x}' \in V(K)}\left(\boldsymbol{u}_h^*(\boldsymbol{x}', t^i)\right) - \min_{\boldsymbol{x}' \in V(K)}\left(\boldsymbol{u}_h^*(\boldsymbol{x}', t^i)\right)\right), \tag{2.98}$$

where $\varepsilon = 10^{-3}$.

Approximation: Evaluate on $\boldsymbol{p}_h^*$, i.e. on the projection to linspace. Projection described in the next chapter.

$$\min_{\boldsymbol{x}' \in V(K)} \boldsymbol{p}_h(\boldsymbol{x}', t^i) - \delta \leq \boldsymbol{p}_h^*(\boldsymbol{x}, t^{i+1}) \leq \max_{\boldsymbol{x}' \in V(K)} \boldsymbol{p}_h(\boldsymbol{x}', t^i) + \delta \tag{2.99}$$

evaluate in terms of subcell averages.

$$\boldsymbol{p}_h^*(\boldsymbol{x}, t^{i+1}) = \boldsymbol{\mathcal{P}}\left(\boldsymbol{u}_h^*(\boldsymbol{x}, t^{i+1})\right) \tag{2.100}$$

as defined in the next section.

MUSCL Hancook

second order total variation diminishing, robust, simple

Consists of three steps:

1. Compute slopes:

$$\left[\delta_d^{K,i}\right]_{\boldsymbol{\alpha},\gamma} = \operatorname{minmod}\left(\left[\hat{\boldsymbol{p}}^{K_L,i}\right]_{\boldsymbol{\alpha}+\boldsymbol{e}_d,\gamma} - \left[\hat{\boldsymbol{p}}^{K_L,i}\right]_{\boldsymbol{\alpha},\gamma}, \left[\hat{\boldsymbol{p}}^{K_L,i}\right]_{\boldsymbol{\alpha},\gamma} - \left[\hat{\boldsymbol{p}}^{K_L,i}\right]_{\boldsymbol{\alpha}-\boldsymbol{e}_d,\gamma}\right) \tag{2.101}$$

for all $\boldsymbol{\alpha} \in \{0,1,\dots,N_S+1\}^D := \boldsymbol{\mathcal{N}}^*_{\boldsymbol{\mathcal{S}}}$, $\gamma \in \mathcal{V}$, unit vectors $\boldsymbol{e}_d$, $d \in \mathcal{D}$, subgrid cells $L^K \in K$, troubled grid cells $K \in \mathcal{K}_h^*$ and $i \in \mathcal{I}$. We furthermore use the common definition of the minmod function, namely

$$\operatorname{minmod}(a,b) = \begin{cases} 0 & \text{if } ab \leq 0 \\ a & \text{if } ab > 0 \text{ and } |a| \leq |b| \\ b & \text{if } ab > 0 \text{ and } |b| < |a|. \end{cases} \tag{2.102}$$

2. Evaluate source:

$$\left[\boldsymbol{s}^{K,i}\right]_{\boldsymbol{\alpha},\gamma} = \left[\boldsymbol{S}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\alpha}\right)\right]_{\gamma} \tag{2.103}$$

for all $\boldsymbol{\alpha} \in \boldsymbol{\mathcal{N}}^*_{\boldsymbol{\mathcal{S}}}$, $\gamma \in \mathcal{V}$, subgrid cells $L^K \in K$, troubled cells $K \in \mathcal{K}_h^*$ and $i \in \mathcal{I}$.

3. Extrapolate:

$$\left[\boldsymbol{w}^{K,i}\right]_{d,e,\boldsymbol{\alpha},\gamma} = \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{\alpha},\gamma} + \frac{e}{2}\left[\delta_d^{K,i}\right]_{\boldsymbol{\alpha},\gamma} \tag{2.104}$$

for $\boldsymbol{\alpha} \in \boldsymbol{\mathcal{N}}^*_{\boldsymbol{\mathcal{S}}}$, $\gamma \in \mathcal{V}$, $d \in \mathcal{D}$ and $e \in \{-1,+1\} := \sigma$, ...

4. Evolve:

$$\left[\boldsymbol{w}^{K,i+\frac{1}{2}}\right]_{d,e,\boldsymbol{\alpha},\gamma} = \frac{\Delta t_i}{2}\sum_{d'\in\mathcal{D}}\sum_{e'\in\sigma}\left(e'\left[\boldsymbol{F}\left(\left[\boldsymbol{w}^{K,i}\right]_{d',e',\boldsymbol{\alpha}}\right)\right]_{\gamma,d'} / \left[\Delta\boldsymbol{x}^{L^K}\right]_{d'}\right) + \frac{\Delta t_i}{2}\left[\boldsymbol{s}^{K,i}\right]_{\boldsymbol{\alpha},\gamma} \tag{2.105}$$

for all $\boldsymbol{\alpha} \in \boldsymbol{\mathcal{N}}^*_{\boldsymbol{\mathcal{S}}}$, $\gamma \in \mathcal{V}$, $d \in \mathcal{D}$, $e \in \sigma$, ...

5. Solve Riemann problems:

$$\left[\boldsymbol{f}^{K,i}\right]_{d,\boldsymbol{\alpha},\gamma} = \left[\boldsymbol{\mathcal{G}}\left(\left[\boldsymbol{w}^{K,i+\frac{1}{2}}\right]_{d,+1,\boldsymbol{\alpha}-\boldsymbol{e}_d}, \left[\boldsymbol{w}^{K,i+\frac{1}{2}}\right]_{d,-1,\boldsymbol{\alpha}+\boldsymbol{e}_d}, \boldsymbol{e}_d\right)\right]_{\gamma} \tag{2.106}$$

6. Evolve source

$$\begin{aligned} \left[\boldsymbol{s}^{K,i+\frac{1}{2}}\right]_{\boldsymbol{\alpha},\gamma} = [\boldsymbol{s}K,i]_{\boldsymbol{\alpha},\gamma} + \\ \frac{1}{2}\sum_{d'\in\mathcal{D}}\sum_{e'\in\sigma}\left(e'\left[\boldsymbol{F}\left(\left[\boldsymbol{w}^{K,i}\right]_{d',e',\boldsymbol{\alpha}}\right)\right]_{\gamma,d'} / \left[\Delta\boldsymbol{x}^{L^K}\right]_{d'}\right) + \\ \frac{1}{2}\left[\boldsymbol{s}^{K,i}\right]_{\boldsymbol{\alpha},\gamma} \end{aligned} \tag{2.107}$$

7. Update solution

$$\begin{aligned} \left[\boldsymbol{p}^{L^K,i+1}\right]_{\boldsymbol{\alpha},\gamma} = \\ \left[\boldsymbol{p}^{L^K,i}\right]_{\boldsymbol{\alpha},\gamma} - \\ \Delta t_i \sum_{d\in\mathcal{D}}\left(\left[f^{K,i}\right]_{d,\boldsymbol{\alpha}+\boldsymbol{e}_d,\gamma} - \left[f^{K,i}\right]_{d,\boldsymbol{\alpha},\gamma} / \left[\Delta\boldsymbol{x}^{L^K}\right]_{d}\right) + \\ \Delta t_i\left[\boldsymbol{s}^{K,i+\frac{1}{2}}\right]_{\boldsymbol{\alpha},\gamma} \end{aligned} \tag{2.108}$$

2.2 Profiling and Energy-aware Computing

Chapter 3

A profiling infrastructure for ExaHyPE

- General architecture
- Architecture profiling
- Functionality

Chapter 4

Preliminary profiling results, case studies

- Analytic benchmark: Introduction, derivation
- Pie-chart per kernel
- Case-study: Cache-misses, compile-time ($\rightarrow$ Toolkit philosophy)
- Degree $\rightarrow$ Wallclock, Energy (AMR)
- Static mesh Δx $\rightarrow$ Error for polynomials (convergence tables)

Chapter 5

Conclusion and Outlook

- PA is important
- ExaHyPE as an answer to exascale challenges
- Applications

Chapter 6

Acknowledgment