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

Master's Thesis in Computational Science and Engineering

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I hereby declare that this thesis is entirely the result of my own work except where otherwise indicated. I have only used the resources given in the list of references.

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Abstract

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2.1.1 Introduction

As stated already in the introduction, the ExaHyPE project is concerned with building an engine for simulating problems that can be formulated in terms of a hyperbolic balance law (HBL). Leaving all of the high performance computing (HPC) components aside, the very heart of the framework therefore comprise of an embedded numerical scheme for solving partial differential equations of HBL type.

Solving PDEs of this kind is both of great interest in practice and has been a topic of active research for about a century[1]. A comprehensive overview on schemes that have been proposed over the years can be found in [7]. Two particularly challenging aspects of such simulations are

1. the accurate simulation of HBL problems over long periods of time, especially when facing (prescribed or spontaneously arising) discon-

[1]The British scientist and Durham University alumnus Lewis Fry Richardson is considered to be one of the founding fathers of computational fluid dynamics (CFD). In 1922 he published a book in which he presents a method for weather forecasting based on the solution of differential equations, in a time when most computations were still done by human "computers". See [6] for a second edition of the book published in 2007 which puts the work into a contemporary context and emphasizes how modern weather forecasting is still based on Richardson's ideas.

tinuities ("shocks") or stiff source terms leading to stability issues in space and time, respectively, and,

2. the inherent data access patterns that numerical schemes inherit from the PDE make it challenging to avoid excessive communication and to achieve high arithmetic density, two key drivers for good performance on modern distributed HPC systems.

In ExaHyPE a state of the art method called Arbitrary High Order Derivatives Discontinuous Galerkin (ADER-DG) scheme is employed together with a-posteriori subcell limiting based on the robust, second-order MUSCL-Hancock finite volume method (FVM) scheme (see [3] for details). As the name implies the Discontinuous Galerkin framework with high order local polynomials ansatz functions acts as the theoretical foundation of the method. In the following sections we will step by step derive the complete scheme and emphasize how it addresses the challenges stated above. The first part on unlimited ADER-DG is based to varying degree on work presented in [1] with three important additional contributions:

1. The scheme is presented in a more general form for systems involving V quantities in D spatial dimensions.
2. We employ index notation and simplify the equations up to a point where the resulting mathematical formulae can easily be mapped to a programming language, in particular it is in direct agreement with FORTRAN code used by Dumbser et al. to generate the numerical results presented in [2].
3. We extend the formulation to include a posteriori subcell limiting, projection and reconstruction operations to equidistant subgrids and introduce the MUSCL-Hancock FVM scheme.

The chapter is set up as follows: First, we will begin with some remarks on the notation employed and state the problem at hand in its general form. Second, we will derive an element local weak formulation and approximate it with respect to finite-dimensional function spaces. After introducing reference coordinates, corresponding mappings and orthogonal bases for the function spaces involved we employ a predictor-corrector approach to arrive at a fully-discrete method that is of arbitrarily hight order in space and time.

2.1.2 Notation

Before we begin deriving the numerical schemes let us quickly introduce the following set of rules on how to depict common mathematical objects and operations:

- Vectors and vector-valued functions, i.e. first-order tensors, will be denoted by bold, lower case letters, e.g. $\boldsymbol{x}$, $\boldsymbol{u}(\boldsymbol{x}, t)$.

- Matrices or matrix-valued functions, i.e. second-order tensors, will be denoted by bold, upper case letters, e.g. $\boldsymbol{K}$, $\boldsymbol{F}(\boldsymbol{x}, t)$.
- Higher order tensors are always denoted as bold, lower-case letters with a "hat" on top, e.g. $\hat{\boldsymbol{u}}^{K,i}$, $\hat{\boldsymbol{q}}^{K,i}$. Note, however, that the opposite is not true[2].
- To avoid confusion in case we deal with tensors for which a superscript or a subscript is "part of its name" or where this indicates membership in a set, similar to the convention in many programming languages, we denote "accesses" into the tensor by square brackets. An example illustrating the advantage of this notation based on common naming conventions in literature could be the following: Let $\{\tilde{\boldsymbol{u}}_h^{K,i}\}_{K\in\mathcal{K}_h, i\in\{0,1,\ldots,I-1\}}$ be the set of vector-valued functions from an appropriate Hilbert space which are defined locally on a cell $K \in \mathcal{K}_h$ and in a time interval $[t_i, t_i + \Delta t_i]$, $i \in \{0, 1, \ldots, I\}$. If we now want the v-th component $\hat{\boldsymbol{u}}^{K,i}$ we write
$$\left[\tilde{\boldsymbol{u}}_h^{K,i}\right]_v \tag{2.1}$$
instead of
$$\tilde{\boldsymbol{u}}_{h,v}^{K,i}. \tag{2.2}$$
In this way it clear that K, i and h are "part of the name" and that v is an index used to access an element in the tensor. However if an expression is absolutely unambiguous, for the sake of brevity, in this case we will often omit the square brackets. Most prominently we write
$$\frac{\partial}{\partial x_d} \tag{2.3}$$
instead of
$$\frac{\partial}{\partial\, [\boldsymbol{x}]_d}. \tag{2.4}$$

- Throughout the thesis we use index notation following the Einstein summation convention whenever possible. This means that if an index within a product expression is repeated exactly once, this implies summation over the whole range of this index. The standard inner product of two vectors $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^N$ can then be written as
$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \sum_{n=0}^{N-1} [\boldsymbol{x}]_n [\boldsymbol{y}]_n = [\boldsymbol{x}]_n [\boldsymbol{y}]_n \,(= [\boldsymbol{x}]_m [\boldsymbol{y}]_m) \tag{2.5}$$

[2] In general the dimensionality of an objects will always be visible from its indices and since we will only allow scalar and vector indices only this distinction is of critical importance.

and for unambiguous cases like above

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \sum_{n=0}^{N-1} x_n y_n := x_n y_n (= x_m y_m). \tag{2.6}$$

Such indices are called dummy indices in the sense that as illustrated in the example above it does not matter if the index is named n or m. Sometimes free indices, i.e. indices that are not dummy indices, appear twice in a term as a result of some algebraic manipulation. In these cases we will explicitly state that summation over the index is not intended, unless it is obvious e.g. from the left-hand side of the equation that the index can only be a free index. We furthermore always give an explicit range for free indices. See [5] for more details on index notation, its advantages and disadvantages as well as a more formal definition.

In addition to increased brevity, index notation allows for less ambiguities compared to classical vector notation, simplifies derivation of identities from tensor calculus and if done carefully the resulting formulae can be conveniently mapped to loops in low-level programming languages such as C or FORTRAN.

- To keep all derivations dimension-agnostic, we define accesses into tensors using vector indices as follows: Let $\hat{\boldsymbol{u}} \in \mathbb{R}^{I_1 \times I_2 \times \ldots \times I_D}$ a tensor of order $D \in \mathbb{N}$ with $I_d \in \mathbb{N}_0$ for all $d \in \{0, 1, \ldots, D-1\} := \mathcal{D}$. Let furthermore $i_d \in \{0, 1, \ldots, I_d - 1\}$ for all $d \in \mathcal{D}$ and $\boldsymbol{i} \in \mathbb{N}_0^D$, $[\boldsymbol{i}]_d = i_d$ for $d \in \mathcal{D}$ a vector of indices. Then we define

$$[\hat{\boldsymbol{u}}]_{\boldsymbol{i}} = [\hat{\boldsymbol{u}}]_{[i_0, i_1, \ldots, i_{D-1}]} = [\hat{\boldsymbol{u}}]_{i_0, i_1, \ldots, i_{D-1}}. \tag{2.7}$$

  If we only provide a vector of $D-1$ indices, i.e.

$$[\hat{\boldsymbol{u}}]_{[i_0, i_1, \ldots, i_{D-2}]}, \tag{2.8}$$

  we obtain a vector of length I_{D-1}. If we only provide $D-2$ indices we obtain a matrix with I_{D-2} rows and I_{D-1} columns. In general if we provide $d \in \{0, 1, \ldots, D\}$ indices we obtain a tensor of order $D - d$.

- In the style of numerical computing environments such as MATLAB® or Octave (see [4]) we define the following shorthand notation for sequences of consecutive integral numbers:

$$j{:}k := \begin{cases} \{j, j+1, \ldots, k\} & \text{if } j \leq k \\ \{\} & \text{otherwise.} \end{cases} \tag{2.9}$$

- We can now define access into a vector $\boldsymbol{x} \in \mathbb{R}^N$ of length N via sequences as

$$[\boldsymbol{x}]_{j:k} := \left[[\boldsymbol{x}]_j, [\boldsymbol{x}]_{j+1}, \ldots, [\boldsymbol{x}]_k \right] \tag{2.10}$$

for $j \leq k$ and $j, k \in 0\!:\!N-1$, which for unambiguous cases as above is equal to the definition

$$\boldsymbol{x}_{j:k} := [x_j, j_{j+1}, \dots, x_k]. \tag{2.11}$$

Together with implicit set and vector concatenation we can then write for $k \in 0 : N-1$

$$[\boldsymbol{x}]_{\{0:k-1,k+1:N-1\}} = \boldsymbol{x}_{\{0:k-1,k+1:N-1\}} \tag{2.12}$$

to denote the vector of length $N-1$ that contains all values of the original vector $\boldsymbol{x}$ but the k-th component. Furthermore

$$\Big[[\boldsymbol{x}]_{0:k-1}, x', [\boldsymbol{x}]_{k+1:N-1}\Big] = \Big[\boldsymbol{x}_{0:k-1}, x', \boldsymbol{x}_{k+1:N-1}\Big] \tag{2.13}$$

denotes the vector of length N whose components are equal to the ones of $\boldsymbol{x}$ apart from the k-th one, which we have replaced by the scalar $x' \in \mathbb{R}$.

2.1.3 Hyperbolic Conservation Laws

A D-dimensional balance law in a system with V quantities is described mathematically by a partial differential equation (PDE) of the form

$$\frac{\partial}{\partial t}\Big[\boldsymbol{u}(\boldsymbol{x},t)\Big]_v + \frac{\partial}{\partial x_d}\Big[\boldsymbol{F}\left(\boldsymbol{u}(\boldsymbol{x},t)\right)\Big]_{vd} = \Big[\boldsymbol{s}\left(\boldsymbol{u}(\boldsymbol{x},t)\right)\Big]_v \text{ on } \boldsymbol{\Omega} \times [0,T] \tag{2.14}$$

together with initial conditions

$$\big[\boldsymbol{u}(\boldsymbol{x},0)\big]_v = \big[\boldsymbol{u}_0(\boldsymbol{x})\big]_v \quad \forall \boldsymbol{x} \in \boldsymbol{\Omega}, \tag{2.15}$$

and boundary conditions

$$\big[\boldsymbol{u}(\boldsymbol{x},t)\big]_v = \big[\boldsymbol{u}_B(\boldsymbol{x},t)\big]_v \quad \forall \boldsymbol{x} \in \partial\boldsymbol{\Omega}, t \in [0,T], \tag{2.16}$$

for all $v \in \mathcal{V}$, where we define the index set $\mathcal{V} = \{1, 2, \dots, V\}$. $[0,T]$ is the time interval of interest and $\boldsymbol{\Omega} \subset \mathbb{R}^D$ denotes the spatial domain. The function $\boldsymbol{F} : \mathbb{R}^V \to \mathbb{R}^{V\times D}, \boldsymbol{u} \mapsto \boldsymbol{F}(\boldsymbol{u}) = \big[\boldsymbol{f}_1(\boldsymbol{u}), \boldsymbol{f}_2(\boldsymbol{u}), \dots, \boldsymbol{f}_D(\boldsymbol{u})\big]$ is called the flux function. For the problem to be hyperbolic we require that all Jacobian matrices $\boldsymbol{A}_d(\boldsymbol{u})$, $d \in \{0, 1, \dots, D-1\} := \mathcal{D}$, defined as

$$[\boldsymbol{A}_d]_{ij} = \frac{\partial\left[\boldsymbol{f}_d\right]_i}{\partial u_j}, \tag{2.17}$$

have D real eigenvalues in each admissible state $\boldsymbol{u} \in \mathbb{R}^V$.

2.1.4 Space and Time Discretization

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

$$K \cap J = \emptyset \forall K, J \in \mathcal{K}_h, K \neq J, \tag{2.18}$$

$$\bigcup_{K \in \mathcal{K}_h} K = \mathbf{\Omega}. \tag{2.19}$$

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

$$0 = t_0 < t_1 < \dots < t_I = T. \tag{2.20}$$

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

$$\Delta t_i = t_{i+1} - t_i, \tag{2.21}$$

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

Without loss of generality we can solve the original PDE (2.14) on $\mathbf{\Omega} \times [0, T]$ simply by solving the PDE locally for each element $K \in \mathcal{K}_h$ in the time interval $[t_0, t_0 + \Delta t_0]$ and then proceeding to the next time interval until we have reached the final time T. This gives rise to an element-local formulation on a subinterval in time which we will focus in the following.

2.1.5 Element-local weak formulation

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

$$L^2(\mathbf{\Omega})^V = \left\{ \boldsymbol{w} : \mathbf{\Omega} \to \mathbb{R}^V \mid \int_{\mathbf{\Omega}} \|\boldsymbol{w}\|^2 \, d\boldsymbol{x} < \infty \right\}. \tag{2.22}$$

Let $\boldsymbol{w} \in L^2(\mathbf{\Omega})^V$ be a spatial test function. Multiplication of the original PDE (2.14) and integration over a space-time cell $K \times [t_i, t_i + \Delta t_i]$ yields a element-local weak formulation of the problem,

$$\begin{aligned} &\int_{t_i}^{t_i+\Delta t_i} \int_K \frac{\partial}{\partial t} [\boldsymbol{u}]_v [\boldsymbol{w}]_v \, d\boldsymbol{x} dt + \int_{t_i}^{t_i+\Delta t_i} \int_K \frac{\partial}{\partial x_d} [\boldsymbol{F}(\boldsymbol{u})]_{vd} [\boldsymbol{w}]_v \, d\boldsymbol{x} dt = \\ &\int_{t_i}^{t_i+\Delta t_i} \int_K [\boldsymbol{s}(\boldsymbol{u})]_v [\boldsymbol{w}]_v \, d\boldsymbol{x} dt, \end{aligned} \tag{2.23}$$

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

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

$$\begin{aligned} &\int_K \frac{\partial}{\partial x_d} [\boldsymbol{F}(\boldsymbol{u})]_{vd} [\boldsymbol{w}]_v \, d\boldsymbol{x} = \\ &\int_K \frac{\partial}{\partial x_d} \left([\boldsymbol{F}(\boldsymbol{u})]_{vd} [\boldsymbol{w}]_v \right) d\boldsymbol{x} - \int_K [\boldsymbol{F}(\boldsymbol{u})]_{vd} \frac{\partial}{\partial x_d} [\boldsymbol{w}]_v \, d\boldsymbol{x}. \end{aligned} \tag{2.24}$$

Application of the divergence theorem to the first term on the right-hand side of (2.24) yields

$$\int_K \frac{\partial}{\partial x_d}\left(\left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd}\left[\boldsymbol{w}\right]_v\right)\,d\boldsymbol{x} = \int_{\partial K}\left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd}\left[\boldsymbol{w}\right]_v\left[\boldsymbol{n}\right]_d\,ds(\boldsymbol{x}), \tag{2.25}$$

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. (2.24) and (2.25) into eq. (2.23) yields the following more favorable element-local weak formulation of the original equation (2.14):

$$\begin{aligned}&\int_{t_i}^{t_i+\Delta t_i}\int_K \frac{\partial}{\partial t}\left[\boldsymbol{u}\right]_v\left[\boldsymbol{w}\right]_v\,d\boldsymbol{x}dt - \int_{t_i}^{t_i+\Delta t_i}\int_K\left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd}\frac{\partial}{\partial x_d}\left[\boldsymbol{w}\right]_v\,d\boldsymbol{x}dt+\\&\int_{t_i}^{t_i+\Delta t_i}\int_{\partial K}\left[\boldsymbol{F}(\boldsymbol{u})\right]_{vd}\left[\boldsymbol{w}\right]_v\left[\boldsymbol{n}\right]_d\,ds(\boldsymbol{x})dt = \int_{t_i}^{t_i+\Delta t_i}\int_K\left[\boldsymbol{s}(\boldsymbol{u})\right]_v\left[\boldsymbol{w}\right]_v\,d\boldsymbol{x}dt.\end{aligned} \tag{2.26}$$

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 $i \in \mathcal{I}$.

2.1.6 Restriction to Finite-Dimensional Function Spaces

To discretize eq. (2.26) we need to impose the restriction that both test and ansatz functions come from a finite-dimensional function 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 than N in each variable on K and $K \times [t_i, t_i + \Delta t_i]$, respectively. We can then define the following finite-dimensional function spaces:

- For spatial functions we define

$$\mathbb{W}_h = \left\{\boldsymbol{w}_h \in L^2(\boldsymbol{\Omega})^V \mid \left.\boldsymbol{w}_h\right|_K := \boldsymbol{w}_h^K \in \mathbb{Q}_N(K)^V\ \forall K \in \mathcal{K}_h\right\}. \tag{2.27}$$

- For space-time functions on the time subinterval $[t_i, t_i + \Delta t_i]$, $i \in \mathcal{I}$ we define

$$\begin{aligned}\tilde{\mathbb{W}}_h^i = \Big\{&\tilde{\boldsymbol{w}}_h^i \in L^2\left(\boldsymbol{\Omega} \times [t_i, t_i + \Delta t_i]\right) \mid \\ &\left.\tilde{\boldsymbol{w}}_h^i\right|_K := \tilde{\boldsymbol{w}}_h^{K,i} \in \mathbb{Q}_N\left(K \times [t_i, t_i + \Delta t_i]\right)\ \forall K \in \mathcal{K}_h\Big\}.\end{aligned} \tag{2.28}$$

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. (2.26), i.e. restricting ourselves to test and ansatz functions from finite-dimensional function spaces, yields an approximation of the weak formulation,

$$\int_{t_i}^{t_i+\Delta t_i} \int_K \frac{\partial}{\partial t} \left[\tilde{\boldsymbol{u}}_h^{K,i}\right]_v \left[\boldsymbol{w}_h^K\right]_v dxdt - \int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{F}(\tilde{\boldsymbol{u}}_h^{K,i})\right]_{vd} \frac{\partial}{\partial x_d} \left[\boldsymbol{w}_h^K\right]_v dxdt +$$
$$\int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{\mathcal{G}}(\tilde{\boldsymbol{u}}_h^{K,i}, \tilde{\boldsymbol{u}}_h^{K^+i}, \boldsymbol{n})\right]_v \left[\boldsymbol{w}_h^K\right]_v ds(\boldsymbol{x})dt =$$
$$\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{s}(\tilde{\boldsymbol{u}}_h^{K,i})\right]_v \left[\boldsymbol{w}_h^K\right]_v dxdt, \tag{2.29}$$

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

$$\tilde{\boldsymbol{u}}_h^{K,i}(\boldsymbol{x}^*) \neq \tilde{\boldsymbol{u}}_h^{K'i}(\boldsymbol{x}^*) \tag{2.30}$$

for $\boldsymbol{x}^* \in K \cap K'$, 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.

Excursus: The Riemann Problem

Let $\boldsymbol{x}^*$ be a point on interface ∂K between a cell $K \in \mathcal{K}_h$ and its Voronoi neighbor $K' \in V(K)$ 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")

$$\frac{\partial}{\partial t} \left[\boldsymbol{g}\right]_v + \sum_{d=1}^{D} \frac{\partial}{\partial x_d} \left[\boldsymbol{F}(\boldsymbol{g})\right]_{vd} \left[\boldsymbol{n}\right]_d = 0 \tag{2.31}$$

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

$$\boldsymbol{g}(\boldsymbol{x}^* + \alpha\boldsymbol{n}, 0) = \begin{cases} \tilde{\boldsymbol{u}}_h^{K,i}\Big|_{\boldsymbol{x}^*} & \text{if } \alpha < 0 \\ \tilde{\boldsymbol{u}}_h^{K',i}\Big|_{\boldsymbol{x}^*} & \text{if } \alpha > 0. \end{cases} \tag{2.32}$$

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

$$\left[\boldsymbol{\mathcal{G}}\left(\tilde{\boldsymbol{u}}_h^{K,i}, \tilde{\boldsymbol{u}}_h^{K',i}, \boldsymbol{n}\right)\right]_v := \left[\tilde{\boldsymbol{g}}\big|_0\right]_v. \tag{2.33}$$

TODO: In practice use approximate Riemann solvers. See bla for an overview on state of the art approximate Riemann solvers.

Continuing with eq. (2.29), integration by parts in time of the first term and noting that $\boldsymbol{w}_h$ is constant in time yields the following one-step update scheme for the cell-local time-discrete solution $\tilde{\boldsymbol{u}}_h^{K,i}$:

$$
\begin{aligned}
\int_K \left[\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i+\Delta t_i} \right]_v \left[\boldsymbol{w}_h^K\right]_v d\boldsymbol{x} = \int_K \left[\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i} \right]_v \left[\boldsymbol{w}_h^K\right]_v d\boldsymbol{x} + \\
\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{u}}_h^{K,i})\right]_{vd} \frac{\partial}{\partial x_d}\left[\boldsymbol{w}_h^K\right]_v d\boldsymbol{x}dt - \\
\int_{t_i}^{t_i+\Delta t_i}\int_{\partial K} \left[\boldsymbol{\mathcal{G}}(\tilde{\boldsymbol{u}}_h^{K,i}, \tilde{\boldsymbol{u}}_h^{K^+i}, \boldsymbol{n})\right]_v \left[\boldsymbol{w}_h^K\right]_v ds(\boldsymbol{x})dt + \\
\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{s}(\tilde{\boldsymbol{u}}_h^{K,i})\right]_v \left[\boldsymbol{w}_h^K\right]_v d\boldsymbol{x}dt.
\end{aligned}
\tag{2.34}
$$

Again we require eq. (2.34) to hold for all $v \in \mathcal{V}$, $\boldsymbol{w}_h \in \mathbb{W}_h$, $K \in \mathcal{K}_h$ and $i \in \mathcal{I}$. Note, however, that the scheme is incomplete, since we only know $\tilde{\boldsymbol{u}}_h^i|_t$ at the discrete time steps $t \in \{t_i, t_i + \Delta t_i\}$, not within the open interval, i.e. for $t \in (t_i, t_i + \Delta t_i)$. As commonly done in a DG framework we therefore proceed by replacing $\tilde{\boldsymbol{u}}_h$ on the interval $(t_i, t_i + \Delta t_i)$ by an approximation $\tilde{\boldsymbol{q}}_h^i \in \tilde{\mathbb{W}}_h^i$ which we call space-time predictor.

2.1.7 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 (2.14), 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 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. (2.25) we obtain the following relation:

$$
\begin{aligned}
&\int_{t_i}^{t_i+\Delta t_i}\int_K \frac{\partial}{\partial t}\left[\tilde{\boldsymbol{q}}_h^{K,i}\right]_v \left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_v d\boldsymbol{x}dt - \\
&\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{q}}_h^{K,i})\right]_{vd} \frac{\partial}{\partial x_d}\left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_v d\boldsymbol{x}dt + \\
&\int_{t_i}^{t_i+\Delta t_i}\int_{\partial K} \left[\boldsymbol{\mathcal{G}}\left(\tilde{\boldsymbol{q}}_h^{K,i}, \tilde{\boldsymbol{q}}_h^{K^+i}, \boldsymbol{n}\right)\right]_v \left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_v ds(\boldsymbol{x})dt = \\
&\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{s}\left(\tilde{\boldsymbol{q}}_h^{K,i}\right)\right]_v \left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_v d\boldsymbol{x}dt.
\end{aligned}
\tag{2.35}
$$

We require eq. (2.35) 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 cells $K \in \mathcal{K}_h$ allows us to drop the third term. Together with integration by parts in time applied to the first term this yields

$$\int_K \left[\tilde{\boldsymbol{q}}_h^{K,i}\Big|_{t_i+\Delta t_i}\right]_v \left[\tilde{\boldsymbol{w}}_h^{K,i}\Big|_{t_i+\Delta t_i}\right]_v d\boldsymbol{x} - \int_{t_i}^{t_i+\Delta t_i}\int_K \left[\tilde{\boldsymbol{q}}_h^{K,i}\right]_v \frac{\partial}{\partial t}\left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_v d\boldsymbol{x}dt =$$
$$\int_K \left[\tilde{\boldsymbol{q}}_h^{K,i}\Big|_{t_i}\right]_v \left[\tilde{\boldsymbol{w}}_h^{K,i}\Big|_{t_i}\right]_v d\boldsymbol{x} + \int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{q}}_h^{K,i})\right]_{vd} \frac{\partial}{\partial x_d}\left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_v d\boldsymbol{x}dt +$$
$$\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{s}\left(\tilde{\boldsymbol{q}}_h^{K,i}\right)\right]_v \left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_v d\boldsymbol{x}dt, \tag{2.36}$$

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 $i \in \mathcal{I}$. In conjunction with the initial condition

$$\tilde{\boldsymbol{q}}_h^{K,i}\Big|_{t_i} = \tilde{\boldsymbol{u}}_h^{K,i} \tag{2.37}$$

and an initial guess

$$\tilde{\boldsymbol{q}}_h^{K,i}\Big|_{t} = \tilde{\boldsymbol{u}}_h^{K,i}\ \forall t \in (t_i, t_i + \Delta t_i] \tag{2.38}$$

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. (2.36) and derive a fully-discrete iterative method to compute the cell-local space-time predictor $\tilde{\boldsymbol{q}}_h^{K,i}$.

2.1.8 Reference Elements and Mappings

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

$$\left[\Delta\boldsymbol{x}^K\right]_d = \max_{\boldsymbol{x}\in K}\,[\boldsymbol{x}]_d - \min_{\boldsymbol{x}\in K}\,[\boldsymbol{x}]_d \tag{2.39}$$

and

$$[\boldsymbol{P}_K]_d = \min_{\boldsymbol{x}\in K}\,[\boldsymbol{x}]_d \tag{2.40}$$

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

$$\boldsymbol{\mathcal{X}}_K : \hat{K} \to K, \boldsymbol{\xi} \mapsto \boldsymbol{\mathcal{X}}_K(\boldsymbol{\xi}) = \boldsymbol{x} \tag{2.41}$$

via the relation

$$[\boldsymbol{x}]_d = \left[\boldsymbol{\mathcal{X}}_K(\boldsymbol{\xi})\right]_d = [\boldsymbol{P}_K]_d + [\Delta \boldsymbol{x}]_d \left[\boldsymbol{\xi}\right]_d \tag{2.42}$$

for $d \in \mathcal{D}$ (i.e. no summation on d) 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

$$\mathcal{T}_i : [0, 1] \to [t_i, t_i + \Delta t_i], \tau \mapsto \mathcal{T}_i(\tau) = t_i + \Delta t_i \tau = t \tag{2.43}$$

maps a point $\tau \in [0, 1]$ in reference time to a point $t \in [t_i, t_i + \Delta t_i]$ in global time 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

$$\boldsymbol{\mathcal{X}}_K^{-1} : K \to \hat{K}, \boldsymbol{x} \mapsto \boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x}) = \boldsymbol{\xi} \tag{2.44}$$

are defined via the relation

$$[\boldsymbol{\xi}]_d = \left[\boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x})\right]_d = \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_d} \left([\boldsymbol{x}]_d - [\boldsymbol{P}_K]_d\right) \tag{2.45}$$

for $d \in \mathcal{D}$ 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

$$\left[\frac{\partial \boldsymbol{\mathcal{X}}_K}{\partial \boldsymbol{\xi}}\right]_{dd'} = \frac{\partial \left[\boldsymbol{\mathcal{X}}_K\right]_d}{\partial \xi_{d'}} = \left[\Delta \boldsymbol{x}^K\right]_d \delta_{dd'}, \tag{2.46}$$

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

$$\delta_{dd'} = \begin{cases} 0 & \text{if } d \neq d' \\ 1 & \text{if } d = d'. \end{cases} \tag{2.47}$$

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

$$J_{\boldsymbol{\mathcal{X}}_K} = \|\frac{\partial \boldsymbol{\mathcal{X}}_K}{\partial \boldsymbol{\xi}}\| = \prod_{d=1}^{D} \left[\Delta \boldsymbol{x}^K\right]_d, \tag{2.48}$$

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

Temporal mappings: The inverse temporal mappings are given as

$$\mathcal{T}_i^{-1} : [t_i, t_i + \Delta t_i] \to [0,1], t \mapsto \mathcal{T}_i^{-1}(t) = \frac{t - t_i}{\Delta t_i} = \tau \tag{2.49}$$

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

$$\frac{d\mathcal{T}_i}{\partial \tau} = \Delta t_i = J_{\mathcal{T}_i} \tag{2.50}$$

which again is constant for all $\tau \in [0,1]$.

2.1.9 Orthogonal Bases for the Finite-Dimensional Function Spaces

In section 2.1.6 we introduced finite-dimensional, cell-wise polynomial function spaces $\mathbb{W}_h$ and $\tilde{\mathbb{W}}_h^i$ for spatial and space-time ansatz and test functions, respectively. On our way towards a fully discrete version of the relations (2.36) and (2.34) to obtain the space-time predictor and the solution at the next time step, respectively, we will now derive a set of functions that form bases for the two function spaces of interest. Following the approach presented by Dumbers et al. in **??**, throughout the thesis we will use the set of Lagrange functions with nodes located at the roots of the Legendre polynomials and tensor products thereof. In the later chapters of this work it will become obvious why this particular choice is highly favorable. For the moment the two major reasons shall be stated as an outlook:

1. Numerical integration using the Gauss-Legendre method is simple and computationally cheap, since the function values at the Gauss-Legendre nodes are directly available as they are equal to the degrees of freedom representing the local polynomial.
2. The resulting bases are orthogonal, which in turn makes sure that the resulting DG-matrices exhibit a spares block structure allowing computations to be carried out efficiently in a dimension-by-dimension manner.

Lagrange Interpolation

Let $f \in \mathbb{Q}_N([0,1])$ be a polynomial of degree less or equal than 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 $[0,1]$. Then the Lagrange interpolation of f,

$$\hat{f}(\xi) = \sum_{n=0}^{N} L_n(\xi) f(\xi_n) \tag{2.51}$$

with Lagrange functions

$$L_n(\xi) = \prod_{m=0, m\neq n}^{N} \frac{\xi - \hat{\xi}_m}{\hat{\xi}_n - \hat{\xi}_m} \tag{2.52}$$

is exact, i.e.

$$f(\xi) = \hat{f}(\xi) \quad \forall \xi \in [0,1]. \tag{2.53}$$

Since therefore every polynomial $f \in \mathbb{Q}_N([0,1])$ can be represented as a linear combination of the Legendre polynomials L_n, $n \in \mathcal{N}$, 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:

$$L_n(\hat{\xi}_{n'}) = \delta_{nn'}, \tag{2.54}$$

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:

$$P_{N+1}(\xi) = \frac{1}{N+1}\left((2N+1)P_N(\xi) - nP_{N-1}(\xi)\right). \tag{2.55}$$

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

$$\hat{\xi}_n = \frac{1}{2}(\tilde{\xi}_n + 1) \tag{2.56}$$

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.

$$\int_0^1 f(\xi)\, d\xi = \sum_{n=0}^{N} \hat{\omega}_n f(\hat{\xi}_n) \quad \forall f \in \mathbb{Q}_{2N+1}\left([0,1]\right). \tag{2.57}$$

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

Scalar-valued Basis Functions on the One-dimensional Reference Element

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.

$$\hat{\psi}_n(x) = \sum_{n'=0}^{N} \frac{x - \hat{x}_{n'}}{\hat{x}_n - \hat{x}_{n'}} \tag{2.58}$$

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

$$\left\langle \hat{\psi}_n, \hat{\psi}_m \right\rangle_{L^2([0,1])} = \int_0^1 \hat{\psi}_n(x)\hat{\psi}_m(x)\, d\boldsymbol{x} = \sum_{n'=0}^{N} \hat{w}'_n \hat{\psi}_n(\hat{x}_{n'})\hat{\psi}_m(\hat{x}_{n'}) = \hat{w}_n \delta_{mn} \tag{2.59}$$

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 $\boldsymbol{\mathcal{N}} := \{0, 1, \dots, N\}^D$ 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

$$\hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi}) = \prod_{d=1}^{D} \hat{\psi}_{[\boldsymbol{n}]_d}([\boldsymbol{\xi}]_d) = \hat{\psi}_{[\boldsymbol{n}]_d}([\boldsymbol{\xi}]_d), \tag{2.60}$$

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

$$\left[\hat{\boldsymbol{\xi}}_{\boldsymbol{n}}\right]_d = \hat{\xi}_{[\boldsymbol{n}]_d} \tag{2.61}$$

and

$$\prod_{d=1}^{D} \hat{\omega}_{[\boldsymbol{n}]_d}, \tag{2.62}$$

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

$$\left\langle \hat{\phi}_{\boldsymbol{n}}, \hat{\phi}_{\boldsymbol{m}} \right\rangle_{L^2(\hat{K})} = \int_{\hat{K}} \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi})\hat{\phi}_{\boldsymbol{m}}(\boldsymbol{\xi})\, d\boldsymbol{\xi} = \sum_{\boldsymbol{n}'\in\boldsymbol{\mathcal{N}}} \left(\hat{\omega}_{\boldsymbol{n}'}\hat{\phi}_{\boldsymbol{n}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{n}'})\hat{\phi}_{\boldsymbol{m}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{n}'})\right) = \hat{\omega}_{\boldsymbol{n}}\delta_{\boldsymbol{nm}} \tag{2.63}$$

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:

$$\delta_{\boldsymbol{nm}} = \prod_{d=1}^{D} \delta_{[\boldsymbol{n}]_d [\boldsymbol{m}]_d} = \delta_{[\boldsymbol{n}]_d [\boldsymbol{m}]_d}. \tag{2.64}$$

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

$$\hat{\theta}_{\boldsymbol{n}l}(\boldsymbol{\xi},\tau) = \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi})\hat{\psi}_l(\tau), \tag{2.65}$$

which again is orthogonal, since

$$\left\langle \hat{\theta}_{\boldsymbol{n}l}, \hat{\theta}_{\boldsymbol{m}k} \right\rangle_{L^2\left(\hat{K}\times[0,1]\right)} = \int_0^1 \int_{\hat{K}} \hat{\theta}_{\boldsymbol{n}l}\hat{\theta}_{\boldsymbol{m}k}\, d\boldsymbol{\xi} d\tau = \hat{\omega}_{\boldsymbol{n}}\hat{\omega}_l \delta_{\boldsymbol{nm}}\delta_{lk} \tag{2.66}$$

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

$$\hat{\boldsymbol{\phi}}_{\boldsymbol{n}v} = \hat{\phi}_{\boldsymbol{n}}\boldsymbol{e}_v, \tag{2.67}$$

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

$$[\boldsymbol{e}_v]_{v'} = \delta_{vv'} \tag{2.68}$$

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

$$\begin{aligned} \left\langle \hat{\boldsymbol{\phi}}_{\boldsymbol{n}v}, \hat{\boldsymbol{\phi}}_{\boldsymbol{n}'v'} \right\rangle_{L^2\left(\hat{K}\right)^V} &= \int_{\hat{K}} \left[\hat{\boldsymbol{\phi}}_{\boldsymbol{n}v}\right]_j \left[\hat{\boldsymbol{\phi}}_{\boldsymbol{n}'v'}\right]_j d\boldsymbol{\xi} = \\ \left([\boldsymbol{e}_v]_j [\boldsymbol{e}_{v'}]_j\right) \int_0^1 \int_{\hat{K}} \hat{\phi}_{\boldsymbol{n}}\hat{\phi}_{\boldsymbol{n}'}\, d\boldsymbol{\xi} &= \hat{\omega}_{\boldsymbol{n}}\delta_{\boldsymbol{nn}'}\delta_{vv'} \end{aligned} \tag{2.69}$$

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

$$\hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv}(\boldsymbol{\xi},\tau) = \hat{\theta}_{\boldsymbol{n}l}(\boldsymbol{\xi},\tau)\boldsymbol{e}_v = \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi})\hat{\psi}_l(\tau)\boldsymbol{e}_v \tag{2.70}$$

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

$$\left\langle \hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv}, \hat{\boldsymbol{\theta}}_{\boldsymbol{n}'l'v'} \right\rangle_{L^2\left(\hat{K}\times[0,1]\right)^V} = \int_0^1 \int_{\hat{K}} \left[\hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv}\right]_j \left[\hat{\boldsymbol{\theta}}_{\boldsymbol{n}'l'v'}\right]_j d\boldsymbol{\xi} d\tau = \hat{\omega}_{\boldsymbol{n}} \hat{\omega}_l \delta_{\boldsymbol{n}\boldsymbol{n}'} \delta_{ll'} \delta_{vv'}, \tag{2.71}$$

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.

2.1.10 Basis Functions in Global Coordinates

We can use the mappings derived in ch. 2.1.8 to map the basis functions to global coordinates. For the vector-valued basis functions on a spatial element K we obtain

$$\boldsymbol{\phi}^K_{\boldsymbol{n}v}(\boldsymbol{x}) = \begin{cases} \left(\hat{\boldsymbol{\phi}}_{\boldsymbol{n}v} \circ \boldsymbol{\mathcal{X}}_K^{-1}\right)(\boldsymbol{x}) & \text{if } \boldsymbol{x} \in K \\ 0 & \text{otherwise,} \end{cases} \tag{2.72}$$

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

$$\boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv}(\boldsymbol{x}, t) = \begin{cases} \left(\hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv} \circ \left(\boldsymbol{\mathcal{X}}_K^{-1}, \mathcal{T}_i^{-1}\right)\right)(\boldsymbol{x}, t) & \text{if } \boldsymbol{x} \in K \text{ and } t \in [t_i, t_i + \Delta t_i] \\ 0 & \text{otherwise} \end{cases} \tag{2.73}$$

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

2.1.11 A Fully-discrete Iterative Method for the Space-time Predictor

We recall relation (2.38) for the space-time predictor. Plugging in the initial condition (2.37) yields

$$\begin{aligned} &\int_K \left[\tilde{\boldsymbol{q}}_h^{K,i}\Big|_{t_i+\Delta t_i}\right]_j \left[\tilde{\boldsymbol{w}}_h^{K,i}\Big|_{t_i+\Delta t_i}\right]_j d\boldsymbol{x} - \int_{t_i}^{t_i+\Delta t_i}\int_K \left[\tilde{\boldsymbol{q}}_h^{K,i}\right]_j \frac{\partial}{\partial t}\left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_j d\boldsymbol{x}dt = \\ &\int_K \left[\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i}\right]_j \left[\tilde{\boldsymbol{w}}_h^{K,i}\Big|_{t_i}\right]_j d\boldsymbol{x} + \int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{q}}_h^{K,i})\right]_{jk} \frac{\partial}{\partial x_k}\left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_j d\boldsymbol{x}dt + \\ &\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{s}\left(\tilde{\boldsymbol{q}}_h^{K,i}\right)\right]_j \left[\tilde{\boldsymbol{w}}_h^{K,i}\right]_j d\boldsymbol{x}dt, \end{aligned} \tag{2.74}$$

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:

$$\tilde{\boldsymbol{q}}_h^{K,i} = \left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n}lv} \boldsymbol{\theta}_{\boldsymbol{n}lv}^{Ki}. \tag{2.75}$$

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

$$\left.\tilde{\boldsymbol{u}}_h^{K,i}\right|_{t_i} = \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n}v} \boldsymbol{\phi}_{\boldsymbol{n}v}^{K}, \tag{2.76}$$

where

$$\left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n}v} = \left[\left.\tilde{\boldsymbol{u}}_h^{K,i}\right|_{\left(\boldsymbol{\mathcal{X}}_K(\boldsymbol{\xi}_{\boldsymbol{n}}),t_i\right)}\right]_v. \tag{2.77}$$

Inserting eqs. (2.75) and (2.76) into eq. (2.74) 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:

$$\begin{aligned}
&\underbrace{\int_K \left[\left.\left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{n}lv} \boldsymbol{\theta}_{\boldsymbol{n}lv}^{Ki}\right|_{t_i+\Delta t_i}\right]_j \left[\left.\boldsymbol{\theta}_{\boldsymbol{\alpha}\beta\gamma}^{Ki}\right|_{t_i+\Delta t_i}\right]_j d\boldsymbol{x}}_{\text{S-I}} - \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{n}lv} \boldsymbol{\theta}_{\boldsymbol{n}lv}^{Ki}\right]_j \frac{\partial}{\partial t}\left[\boldsymbol{\theta}_{\boldsymbol{\alpha}\beta\gamma}^{Ki}\right]_j d\boldsymbol{x}dt}_{\text{S-II}} = \\
&\underbrace{\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n}v} \boldsymbol{\phi}_{\boldsymbol{n}v}^{K}\right]_j \left[\left.\boldsymbol{\theta}_{\boldsymbol{\alpha}\beta\gamma}^{Ki}\right|_{t_i}\right]_j d\boldsymbol{x}}_{\text{S-III}} + \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv} \boldsymbol{\theta}_{\boldsymbol{n}lv}^{Ki}\right)\right]_{jk} \frac{\partial}{\partial x_k}\left[\boldsymbol{\theta}_{\boldsymbol{\alpha}\beta\gamma}^{Ki}\right]_j d\boldsymbol{x}dt}_{\text{S-IV}} + \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv} \boldsymbol{\theta}_{\boldsymbol{n}lv}^{Ki}\right)\right]_j \left[\boldsymbol{\theta}_{\boldsymbol{\alpha}\beta\gamma}^{Ki}\right]_j d\boldsymbol{x}dt}_{\text{S-V}}.
\end{aligned} \tag{2.78}$$

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

$$\left[\hat{\boldsymbol{q}}^{K,i,0}\right]_{\boldsymbol{n}vl} = \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n}v} \tag{2.79}$$

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 $K \in \mathcal{K}_h$ and $i \in \mathcal{I}$.

Term S-I

The first term of eq. (2.78) 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{\mathcal{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{\mathcal{X}}_K} \sum_{\boldsymbol{\alpha}' \in \boldsymbol{\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{\mathcal{X}}_K} \sum_{\boldsymbol{\alpha}' \in \boldsymbol{\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{\mathcal{X}}_K} \hat{\omega}_{\boldsymbol{\alpha}} \left[\hat{\psi}_\beta \Big|_1 \hat{\psi}_l \Big|_1 \right] \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{\alpha}l\gamma} = \\
&J_{\boldsymbol{\mathcal{X}}_K} \hat{\omega}_{\boldsymbol{\alpha}} \left[\boldsymbol{R} \right]_{\beta,l} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{\alpha}l\gamma} ,
\end{aligned}
\tag{2.80}
$$

where we remember from eq. (2.48) that

$$
J_{\boldsymbol{\mathcal{X}}_K} = \prod_{d=1}^{D} [\Delta \boldsymbol{x}]_d \tag{2.81}
$$

and we define the matrix $\boldsymbol{R}$ representing the Right Reference Element Mass Operator as

$$
[\boldsymbol{R}]_{i,j} := \left[\hat{\psi}_i \Big|_1 \hat{\psi}_j \Big|_1 \right]_{i,j} \tag{2.82}
$$

for $i, j \in \mathcal{N}$. A Python script to compute $\boldsymbol{R}$ can be found in appendix **??**.

Term S-II

The second term of eq. (2.78) 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{\mathcal{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{\mathcal{X}}_K}\sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}}\sum_{\beta'\in\mathcal{N}}\Bigg(\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 \\
&\qquad\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\Bigg) = \\
&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[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{n}lv}\delta_{\boldsymbol{n}\boldsymbol{\alpha}'}\delta_{l\beta'}\delta_{vj}\dots \\
&\qquad\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}\Bigg) = \\
&J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\hat{\omega}_{\boldsymbol{\alpha}}\frac{1}{\Delta t_i}\sum_{\beta'\in\mathcal{N}}\left(\hat{\omega}_{\beta'}\left[\frac{\partial}{\partial\tau}\hat{\psi}_\beta(\hat{\tau}_{\beta'})\right]\left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{\alpha}\beta'\gamma}\right) = \\
&J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\hat{\omega}_{\boldsymbol{\alpha}}\frac{1}{\Delta t_i}\left[\boldsymbol{K}\right]_{\beta,\beta'}\left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{\alpha}\beta'\gamma}
\end{aligned}
\tag{2.83}
$$

where we remember from eq. (2.50) that

$$J_{\mathcal{T}_i} = \Delta t_i, \tag{2.84}$$

so that Δt_i and $1/\Delta t_i$ in eq. (2.83) cancel. In the derivation we made use of the fact that due to the chain rule

$$\frac{\partial}{\partial t}\psi^i_\beta = \frac{\partial}{\partial t}\left(\hat{\psi}_\beta\circ\mathcal{T}_i^{-1}\right) = \left(\frac{\partial}{\partial\tau}\hat{\psi}_\beta\right)\left(\frac{\partial}{\partial t}\mathcal{T}_i^{-1}\right) = \frac{1}{\Delta t_i}\frac{\partial}{\partial\tau}\hat{\psi}_\beta. \tag{2.85}$$

We furthermore introduce the matrix $\boldsymbol{K}$ representing the Reference Element Stiffness Operator given as

$$\left[\boldsymbol{K}\right]_{ij} = \hat{\omega}_j\frac{\partial}{\partial\tau}\hat{\psi}_i(\hat{\tau}_j) \tag{2.86}$$

for $i,j\in\mathcal{N}$. A Python script to compute $\boldsymbol{K}$ can be found in appendix **??**.

Term S-III

The third term of eq. (2.78) can be rewritten with respect to reference coordinates as follows:

$$
\begin{aligned}
&\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i} \right]_{nv} \boldsymbol{\phi}^K_{nv} \right]_j \left[\boldsymbol{\theta}^{Ki}_{\alpha\beta\gamma} \Big|_{t_i} \right]_j dx = \\
&\int_K \left[\hat{\boldsymbol{u}}^{K,i} \right]_{nv} \phi^K_{\boldsymbol{n}} \left[\boldsymbol{e}_v \right]_j \phi^K_{\boldsymbol{\alpha}} \left(\psi^i_\beta \Big|_{t_i} \right) \left[\boldsymbol{e}_\gamma \right]_j dx = \\
&J\boldsymbol{x}_K \int_{\hat{K}} \left[\hat{\boldsymbol{u}}^{K,i} \right]_{nv} \hat{\phi}_{\boldsymbol{n}} \left[\boldsymbol{e}_v \right]_j \hat{\phi}_{\boldsymbol{\alpha}} \left(\hat{\psi}_\beta \Big|_0 \right) \left[\boldsymbol{e}_\gamma \right]_j d\boldsymbol{\xi} = \\
&J\boldsymbol{x}_K \sum_{\boldsymbol{\alpha}' \in \mathcal{N}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{u}}^{K,i} \right]_{nv} \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'}) \left[\boldsymbol{e}_v \right]_j \hat{\phi}_{\boldsymbol{\alpha}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'}) \left(\hat{\psi}_\beta \Big|_0 \right) \left[\boldsymbol{e}_\gamma \right]_j \right) = \\
&J\boldsymbol{x}_K \sum_{\boldsymbol{\alpha}' \in \mathcal{N}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{u}}^{K,i} \right]_{nv} \delta_{\boldsymbol{n}\boldsymbol{\alpha}'} \delta_{vj} \delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'} \left(\hat{\psi}_\beta \Big|_0 \right) \delta_{\gamma j} \right) = \\
&J\boldsymbol{x}_K \hat{\omega}_{\boldsymbol{\alpha}} \left[\hat{\psi}_\beta \Big|_0 \right] \left[\hat{\boldsymbol{u}}^{K,i} \right]_{\boldsymbol{\alpha}\gamma} = \\
&J\boldsymbol{x}_K \hat{\omega}_{\boldsymbol{\alpha}} \left[\boldsymbol{l} \right]_\beta \left[\hat{\boldsymbol{u}}^{K,i} \right]_{\boldsymbol{\alpha}\gamma},
\end{aligned}
\tag{2.87}
$$

where we define the vector $\boldsymbol{l}$ representing the Left Reference Time Flux Operator as

$$
[\boldsymbol{l}]_i = \hat{\psi}_i \Big|_0 \tag{2.88}
$$

for $i \in \mathcal{N}$. A Python script to compute $\boldsymbol{l}$ can be found in appendix **??**.

Term S-IV

The third term of eq. (2.78) 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{\mathcal{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{\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{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{\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{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{\mathcal{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\hat{\omega}_{\alpha'_k}\left(\frac{\partial}{\partial\xi_k}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\hat{\xi}_{\alpha'_k}\right)\right)\left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\left[[\boldsymbol{\alpha}]_{1:k-1},\alpha'_k,[\boldsymbol{\alpha}]_{k+1:N}\right]}\right)\right]_{jk}\right)\right) = \\
&J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{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[\boldsymbol{K}]_{[\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{2.89}
$$

where we used that

$$\frac{\partial}{\partial x_k}\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma}(\boldsymbol{x},t) = \left(\frac{\partial}{\partial x_k}\phi^K_{\boldsymbol{\alpha}}(\boldsymbol{x})\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma = \left(\frac{\partial}{\partial x_k}\prod_{d=1}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma =$$
$$\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\left(\frac{\partial}{\partial x_k}\psi^K_{[\boldsymbol{\alpha}]_k}([\boldsymbol{x}]_k)\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma =$$
$$\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\left(\frac{\partial}{\partial x_k}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}^{-1}_K(\boldsymbol{x})\right]_k\right)\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma =$$
$$\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\left(\left(\frac{\partial}{\partial \xi_k}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}^{-1}_K(\boldsymbol{x})\right]_k\right)\right)\left(\frac{\partial}{\partial x_k}\left[\boldsymbol{\mathcal{X}}^{-1}_K(\boldsymbol{x})\right]_k\right)\right)\dots$$
$$\dots\psi^i_\beta(t)\boldsymbol{e}_\gamma =$$
$$\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\left(\frac{1}{\left[\Delta\boldsymbol{x}^K\right]_k}\frac{\partial}{\partial \xi_k}\hat{\phi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}^{-1}_K(\boldsymbol{x})\right]_k\right)\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma. \tag{2.90}$$

Term S-V

The fifth term of eq. (2.78) can be rewritten with respect to reference coordinates as follows:

$$\int_{t_i}^{t_i+\Delta t_i}\int_K\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv}\boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv}\right)\right]_j\left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma}\right]_j d\boldsymbol{x}dt =$$
$$J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\int_0^1\int_{\hat{K}}\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv}\hat{\phi}_{\boldsymbol{n}}\hat{\psi}_l\boldsymbol{e}_v\right)\right]_j\hat{\phi}_{\boldsymbol{\alpha}}\hat{\psi}_l\left[\boldsymbol{e}_\gamma\right]_j d\boldsymbol{\xi}d\tau =$$
$$J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}}\sum_{\beta'\in\mathcal{N}}\left(\hat{\omega}_{\boldsymbol{\alpha}'}\hat{\omega}_{\beta'}\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv}\hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'})\hat{\psi}_l(\hat{\tau}_{\beta'})\boldsymbol{e}_v\right)\right]_j\dots\right.$$
$$\left.\dots\hat{\phi}_{\boldsymbol{\alpha}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'})\hat{\psi}_\beta(\hat{\tau}_{\beta'})\left[\boldsymbol{e}_\gamma\right]_j\right) =$$
$$J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}}\sum_{\beta'\in\mathcal{N}}\left(\hat{\omega}_{\boldsymbol{\alpha}'}\hat{\omega}_{\beta'}\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv}\delta_{\boldsymbol{n}\boldsymbol{\alpha}'}\delta_{l\beta'}\boldsymbol{e}_v\right)\right]_j\delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'}\delta_{\beta\beta'}\delta_{\gamma j}\right) =$$
$$J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\hat{\omega}_{\boldsymbol{\alpha}}\hat{\omega}_\beta\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{\alpha}\beta v}\boldsymbol{e}_v\right)\right]_\gamma \tag{2.91}$$

The Complete Fixed-point Iteration

Now collecting the results from eqs. (2.80), (2.83), (2.87), (2.89) and (2.91) and plugging them back into eq. (2.78) and division by $J_{\mathcal{X}_K}$ and $\hat{\omega}_{\boldsymbol{\alpha}}$ yields

$$
\begin{aligned}
&(\boldsymbol{R}-\boldsymbol{K})_{\beta\beta'}\left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{\alpha}\beta'\gamma} = [\boldsymbol{l}]_{\beta}\left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{\alpha}\gamma} + \\
&J_{\mathcal{T}_i}\frac{\hat{\omega}_\beta}{\hat{\omega}_{\boldsymbol{\alpha}}}\sum_{k=1}^{D}\left(\frac{1}{[\Delta \boldsymbol{x}]_k}\sum_{\alpha_k'\in\{0,1,\dots,N\}}\left(\prod_{d=0,d\neq k}^{D}\hat{\omega}_{[\boldsymbol{\alpha}]_d}\dots\right.\right.\\
&\left.\left.\dots[\boldsymbol{K}]_{[\boldsymbol{\alpha}]_k,\alpha_k'}\left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{[\alpha_0,\alpha_1,\dots,\alpha_{k-1},\alpha_k',\alpha_{k+1},\dots,\alpha_N]\beta v}\boldsymbol{e}_v\right)\right]_{\gamma k}\right)\right) + \\
&J_{\mathcal{T}_i}\hat{\omega}_\beta\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{\alpha}\beta v}\boldsymbol{e}_v\right)\right]_{\gamma},
\end{aligned}
\tag{2.92}
$$

which has to hold for all $\boldsymbol{\alpha} \in \boldsymbol{\mathcal{N}}$, $\beta \in \mathcal{N}$ and $\gamma \in \mathcal{V}$. To speed up the computation of the new iterate $\hat{\boldsymbol{q}}^{K,i,r+1}$ we can compute the inverse $(\boldsymbol{R} - \boldsymbol{K})^{-1}$ prior to the simulation. A Python script to compute the matrix can be found in appendix **??**.

A possible termination criterion could be $\Delta < \varepsilon$, where $\varepsilon > 0$ is a suitable constant related to the desired accuracy of the iteration, e.g. $\varepsilon = 10^{-7}$ and the squared element-wise residual Δ^2 is defined as follows:

$$
\Delta^2 = \sum_{\boldsymbol{n}\in\boldsymbol{\mathcal{N}}}\sum_{l\in\mathcal{N}}\sum_{v\in\mathcal{V}}\left(\left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{n},l,v} - \left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n},l,v}\right). \tag{2.93}
$$

For linear homogeneous scalar hyperbolic balance laws and neglecting floating point errors it can be proven that the iteration converges after at most N steps (see **??** for details).

2.1.12 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. (2.34). Inserting the local space-time predictor $\tilde{\boldsymbol{q}}_h^{K,i}$ yields

$$\begin{aligned}
&\int_K \left[\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i+\Delta t_i} \right]_v \left[\boldsymbol{w}_h^K \right]_v d\boldsymbol{x} = \int_K \left[\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i} \right]_v \left[\boldsymbol{w}_h^K \right]_v d\boldsymbol{x} + \\
&\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{q}}_h^{K,i}) \right]_{vd} \frac{\partial}{\partial x_d} \left[\boldsymbol{w}_h^K \right]_v d\boldsymbol{x}dt + \\
&\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{s}\left(\hat{\boldsymbol{q}}^{K,i} \right) \right]_v \left[\boldsymbol{w}_h^K \right]_v d\boldsymbol{x}dt - \\
&\int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{\mathcal{G}}\left(\tilde{\boldsymbol{q}}_h^{K,i}, \tilde{\boldsymbol{q}}_h^{K^+i}, \boldsymbol{n} \right) \right]_v \left[\boldsymbol{w}_h^K \right]_v ds(\boldsymbol{x})dt,
\end{aligned} \tag{2.94}$$

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_i and $t_i + \Delta t_i$ can be represented by tensors of coefficients $\hat{\boldsymbol{u}}^{K,i}$ and $\hat{\boldsymbol{u}}^{K,i+1}$ as

$$\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i} = \left[\hat{\boldsymbol{u}}^{K,i} \right]_{\boldsymbol{n},v} \boldsymbol{\phi}_{\boldsymbol{n},v}^K \tag{2.95}$$

and

$$\tilde{\boldsymbol{u}}_h^{K,i}\Big|_{t_i+\Delta t_i} = \left[\hat{\boldsymbol{u}}^{K,i+1} \right]_{\boldsymbol{n},v} \boldsymbol{\phi}_{\boldsymbol{n},v}^K, \tag{2.96}$$

respectively. Inserting eqs. (2.95) and (2.96) and the ansatz for the space-time predictor (2.75) into eq. (2.94) yields

$$\begin{aligned}
&\underbrace{\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i+1} \right]_{\boldsymbol{n},v} \boldsymbol{\phi}_{\boldsymbol{n},v}^K \right]_j \left[\boldsymbol{\phi}_{\boldsymbol{\alpha},\gamma}^K \right]_j d\boldsymbol{x}}_{\text{U-I}} = \underbrace{\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i} \right]_{\boldsymbol{n},v} \boldsymbol{\phi}_{\boldsymbol{n},v}^K \right]_j \left[\boldsymbol{\phi}_{\boldsymbol{\alpha},\gamma}^K \right]_j}_{\text{U-II}} + \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i} \right]_{\boldsymbol{n},l,v} \boldsymbol{\theta}_{\boldsymbol{n},l,v}^{Ki} \right) \right]_{jk} \frac{\partial}{\partial x_k} \left[\boldsymbol{\phi}_{\boldsymbol{\alpha},\gamma}^K \right]_j d\boldsymbol{x}dt}_{\text{U-III}} + \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i} \right]_{\boldsymbol{n},l,v} \boldsymbol{\theta}_{\boldsymbol{n},l,v}^{Ki} \right) \right]_j \left[\boldsymbol{\phi}_{\boldsymbol{\alpha},\gamma}^K \right]_j d\boldsymbol{x}dt}_{\text{U-IV}} - \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{\mathcal{G}}\left(\hat{\boldsymbol{q}}^{K,i}, \hat{\boldsymbol{q}}^{K^+,i}, \boldsymbol{n} \right) \right]_j \left[\boldsymbol{\phi}_{\boldsymbol{\alpha},\gamma}^K \right]_j ds(\boldsymbol{x})dt}_{\text{U-V}},
\end{aligned} \tag{2.97}$$

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. (2.97) can be rewritten with respect to reference coordinates as follows:

$$
\begin{aligned}
&\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i+1} \right]_{\boldsymbol{n},v} \boldsymbol{\phi}^K_{\boldsymbol{n},v} \right]_j \left[\boldsymbol{\phi}^K_{\boldsymbol{\alpha},\gamma} \right]_j d\boldsymbol{x} = \\
&\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i+1} \right]_{\boldsymbol{n},v} \phi^K_{\boldsymbol{n}} \boldsymbol{e}_v \right]_j \left[\phi^K_{\boldsymbol{\alpha}} \boldsymbol{e}_\gamma \right]_j d\boldsymbol{x} = \\
&J\boldsymbol{x}_K \int_{\hat{K}} \left[\left[\hat{\boldsymbol{u}}^{K,i+1} \right]_{\boldsymbol{n},v} \hat{\phi}_{\boldsymbol{n}} \boldsymbol{e}_v \right]_j \left[\hat{\phi}_{\boldsymbol{\alpha}} \boldsymbol{e}_\gamma \right]_j d\boldsymbol{\xi} = \\
&J\boldsymbol{x}_K \sum_{\boldsymbol{\alpha}' \in \boldsymbol{\mathcal{N}}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{u}}^{K,i+1} \right]_{\boldsymbol{n},v} \hat{\phi}_{\boldsymbol{n}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \left[\boldsymbol{e}_v \right]_j \hat{\phi}_{\boldsymbol{\alpha}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \left[\boldsymbol{e}_\gamma \right]_j \right) = \\
&J\boldsymbol{x}_K \sum_{\boldsymbol{\alpha}' \in \boldsymbol{\mathcal{N}}} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{u}}^{K,i+1} \right]_{\boldsymbol{n},v} \delta_{\boldsymbol{n}\boldsymbol{\alpha}'} \delta_{vj} \delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'} \delta_{\gamma j} \right) = \\
&J\boldsymbol{x}_K \hat{\omega}_{\boldsymbol{\alpha}} \left[\hat{\boldsymbol{u}}^{K,i+1} \right]_{\boldsymbol{\alpha},\gamma} .
\end{aligned}
\tag{2.98}
$$

Term U-II

Analogously to the first term of eq. (2.97), the second term can be rewritten as follows:

$$
\begin{aligned}
&\int_K \left[\left[\hat{\boldsymbol{u}}^{K,i} \right]_{\boldsymbol{n},v} \boldsymbol{\phi}^K_{\boldsymbol{n},v} \right]_j \left[\boldsymbol{\phi}^K_{\boldsymbol{\alpha},\gamma} \right]_j d\boldsymbol{x} = \\
&J\boldsymbol{x}_K \hat{\omega}_{\boldsymbol{\alpha}} \left[\hat{\boldsymbol{u}}^{K,i} \right]_{\boldsymbol{\alpha},\gamma} .
\end{aligned}
\tag{2.99}
$$

Term U-III

The third term of eq. (2.97) 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}dt \\
&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(\left[\boldsymbol{\xi} \right]_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}} \left(\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}(\left[\boldsymbol{\xi}_{\boldsymbol{\alpha}'}\right]_d) \right) \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_k} \frac{\partial}{\partial \xi_k} \hat{\psi} \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{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 \left[\boldsymbol{\alpha}'\right]_d} \right) \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_k} \frac{\partial}{\partial \xi_k} \hat{\psi}_{[\boldsymbol{\alpha}]_k} \left(\left[\boldsymbol{\xi}_{\boldsymbol{\alpha}'}\right]_k \right) \right. \\
&J_{\mathcal{T}_i} J_{\boldsymbol{\mathcal{X}}_K} \hat{\omega}_{\boldsymbol{\alpha}} \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} \frac{\partial}{\partial \xi_k} \hat{\psi}_{\alpha'_k} \left(\left[\hat{\boldsymbol{\xi}}\right]_{\alpha'_k} \right) \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} \right.\right.\right.\right. \\
&J_{\mathcal{T}_i} J_{\boldsymbol{\mathcal{X}}_K} \hat{\omega}_{\boldsymbol{\alpha}} \sum_{k=1}^{D} \left(\sum_{\alpha'_k\in\mathcal{N}} \sum_{\beta'\in\mathcal{N}} \left(\frac{1}{\hat{\omega}_{\alpha'_k}} \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_k} \left[\boldsymbol{K}\right]_{\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.
\end{aligned}
\tag{2.100}
$$

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

$$\frac{\partial}{\partial x_k}\left(\prod_{d=1}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right) = \left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\frac{\partial}{\partial x_k}\psi^K_{[\boldsymbol{\alpha}]_k}([\boldsymbol{x}]_k) =$$
$$\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\frac{\partial}{\partial \xi_j}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}_K(\boldsymbol{x})\right]_k\right)\frac{\partial}{\partial x_k}\left[\boldsymbol{\mathcal{X}}_K(\boldsymbol{x})\right]_j =$$
$$\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\frac{\partial}{\partial \xi_j}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}_K(\boldsymbol{x})\right]_k\right)\frac{1}{\left[\Delta\boldsymbol{x}^K\right]_k}\delta_k j =$$
$$\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\frac{1}{\left[\Delta\boldsymbol{x}^K\right]_k}\frac{\partial}{\partial \xi_k}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}_K(\boldsymbol{x})\right]_k\right) dxdt. \tag{2.101}$$

Term U-IV

The fourth term of eq. (2.97) can be rewritten with respect to reference coordinates as follows:

$$\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v}\boldsymbol{\theta}^{Ki}_{\boldsymbol{n},l,v}\right)\right]_j\left[\boldsymbol{\phi}^K_{\boldsymbol{\alpha},\gamma}\right]_j dxdt =$$
$$\int_{t_i}^{t_i+\Delta t_i}\int_K \left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v}\phi^K_{\boldsymbol{n}}\psi^i_l\boldsymbol{e}_v\right)\right]_j\phi^K_{\boldsymbol{\alpha}}\left[\boldsymbol{e}_\gamma\right]_j dxdt =$$
$$J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\int_0^1\int_{\hat{K}}\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v}\hat{\phi}_{\boldsymbol{n}}\hat{\psi}_l\boldsymbol{e}_v\right)\right]_j\hat{\phi}_{\boldsymbol{\alpha}}\left[\boldsymbol{e}_\gamma\right]_j d\boldsymbol{\xi}d\tau =$$
$$J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}}\sum_{\beta'\in\mathcal{N}}\left(\hat{\omega}_{\boldsymbol{\alpha}'}\hat{\omega}_{\beta'}\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v}\hat{\phi}_{\boldsymbol{n}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'})\hat{\psi}_l(\hat{\tau}_{\beta'}\boldsymbol{e}_v)\right)\right]_j\hat{\phi}_{\boldsymbol{\alpha}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'})\left[\boldsymbol{e}_\gamma\right]_j\right) =$$
$$J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\sum_{\boldsymbol{\alpha}'\in\boldsymbol{\mathcal{N}}}\sum_{\beta'\in\mathcal{N}}\left(\hat{\omega}_{\boldsymbol{\alpha}'}\hat{\omega}_{\beta'}\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{n},l,v}\delta_{\boldsymbol{n}\boldsymbol{\alpha}'}\delta_{l\beta'}\boldsymbol{e}_v)\right)\right]_j\delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'}\delta_{\gamma j}\right) =$$
$$J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\hat{\omega}_{\boldsymbol{\alpha}}\sum_{\beta'\in\mathcal{N}}\left(\hat{\omega}_{\beta'}\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{\alpha},\beta',v}\boldsymbol{e}_v\right)\right]_\gamma\right). \tag{2.102}$$

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

$$\partial\hat{K}_{d,e} = \left\{\boldsymbol{\xi}\in\hat{K} \mid \left[\boldsymbol{\xi}\right]_d = e\right\}, \tag{2.103}$$

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

$$\partial K_{d,e} = \boldsymbol{\mathcal{X}}_K\left(\partial\hat{K}_{d,e}\right), \tag{2.104}$$

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. (2.97) 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{2.105}$$

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

$$\left[\boldsymbol{e}_d\right]_{d'} = \delta_{dd'} \tag{2.106}$$

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

The Complete One-step Update Scheme

Inserting eqs. (2.98) to (2.100), (2.102) and (2.105) into eq. (2.97) and dividing the resulting equation by $\hat{\omega}_{\boldsymbol{\alpha}}$ and $J_{\boldsymbol{\mathcal{X}}_K}$ yields

$$
\begin{aligned}
&\left[\hat{\boldsymbol{u}}^{K,i+1}\right]_{\boldsymbol{\alpha},\gamma} = \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{\alpha},\gamma} + \\
&J_{\mathcal{T}_i} \sum_{k=1}^{D} \left(\sum_{\alpha'_k \in \mathcal{N}} \sum_{\beta' \in \mathcal{N}} \left(\frac{\hat{\omega}_{\beta'}}{\hat{\omega}_{\alpha'_k}} \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_k} \underbrace{\frac{\partial}{\partial \xi_k} \hat{\psi}_{\alpha'_k} \left(\left[\hat{\boldsymbol{\xi}}\right]_{\alpha'_k} \right)}_{\mathrm{Kxi}_{\alpha'_k k}} \left[\boldsymbol{F} \left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\left[[\boldsymbol{\alpha}]_1,[\boldsymbol{\alpha}]_2,\ldots,[\boldsymbol{\alpha}]_{k-1},\alpha'_k,[\boldsymbol{\alpha}]_{k+1},\ldots,[\boldsymbol{\alpha}]_D\right],\beta',v} \boldsymbol{e}_v \right) \right]_{\gamma,k} \right) \right) + \\
&J_{\mathcal{T}_i} \sum_{\beta' \in \mathcal{N}} \left(\hat{\omega}_{\beta'} \left[\boldsymbol{s} \left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\boldsymbol{\alpha},\beta',v} \boldsymbol{e}_v \right) \right]_{\gamma} \right) - \\
&J_{\mathcal{T}_i} \sum_{\beta' \in \mathcal{D}} \sum_{d \in \mathcal{D}} \sum_{e \in \mathcal{E}} \sum_{\alpha'_d \in \mathcal{N}} \left(\frac{\hat{\omega}_{\beta'}}{\hat{\omega}_{\alpha'_d}} \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_d} \left[\boldsymbol{\mathcal{G}} \left(\hat{\boldsymbol{q}}^{K,i}, \hat{\boldsymbol{q}}^{K^+,i}, (-1)^e \boldsymbol{e}_d \right) \right]_{\gamma} \underbrace{\left(\hat{\psi}_{\alpha'_d}\Big|_e \right)}_{\mathrm{F0,\ F1}} \right),
\end{aligned}
\tag{2.107}
$$

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

$$
\Delta t \leq \frac{1}{D} \frac{1}{(2N+1)} \min_{d \in \mathcal{D}} \left(\frac{[\Delta \boldsymbol{x}]_d}{\Lambda^d} \right), \tag{2.108}
$$

where

$$
\Lambda^d = \underset{v \in \mathcal{V}}{\text{maxabs}} \left[\boldsymbol{\lambda}^d \right]_v \tag{2.109}
$$

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

$$
\frac{\partial}{\partial x_j} \left[\boldsymbol{F} \left(\boldsymbol{u}(\boldsymbol{x}, t) \right) \right]_{id} \tag{2.110}
$$

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

2.1.13 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

$$\Delta t \leq \frac{1}{d}\frac{1}{N_S}\min_{d\in\mathcal{D}}\left(\frac{[\Delta \boldsymbol{x}]_d}{\Lambda^d}\right). \tag{2.111}$$

Comparing eq. (2.111) to the time step restriction for the ADER-DG scheme given in eq. (2.108) 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 $L^K_{\boldsymbol{j}}$, $\boldsymbol{j} \in \{1, 2, \dots, (N_S)^D\} := \boldsymbol{\mathcal{N}_S}$ 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:

$$\begin{aligned}
\left[\hat{\boldsymbol{p}}^{K_L,i}\right]_{\boldsymbol{\alpha},\gamma} =& \frac{1}{|L_K^{\boldsymbol{\alpha}}|}\int_{L_K^{\boldsymbol{\alpha}}} \left[\tilde{\boldsymbol{u}}_h^{K,i}\right]_{\gamma} d\boldsymbol{x} = \frac{1}{|L_K^{\boldsymbol{\alpha}}|}\int_{L_K^{\boldsymbol{\alpha}}} \phi_{\boldsymbol{n}}^K(\boldsymbol{x})\left[\boldsymbol{e}_v\right]_{\gamma} d\boldsymbol{x} \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n},v} = \\
& \int_{\hat{K}} \hat{\phi}_{\boldsymbol{n}}\left(\frac{1}{N_S}\boldsymbol{\alpha} + \frac{1}{N_S}\boldsymbol{\xi}\right) d\xi \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n},\gamma} = \\
& \sum_{\alpha' \in \mathcal{N}} \left(\hat{\omega}_{\boldsymbol{\alpha}'}\hat{\phi}_{\boldsymbol{n}}\left(\frac{1}{N_S}\boldsymbol{\alpha} + \frac{1}{N_S}\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}\right)\right)\left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{n},\gamma},
\end{aligned} \tag{2.112}$$

which can be carried out efficiently in a dimension-by-dimension manner. See **??** for details.

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

$$\pi_k\left(\boldsymbol{u}_h^*(\boldsymbol{x}, t^{i+1})\right) > 0 \tag{2.113}$$

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

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

$$\min_{\boldsymbol{x}' \in V(K)} \boldsymbol{u}_h(\boldsymbol{x}', t^i) - \delta \leq \boldsymbol{u}_h^*(\boldsymbol{x}, t^{i+1}) \leq \min_{\boldsymbol{x}' \in V(K)} \boldsymbol{u}_h(\boldsymbol{x}', t^i) + \delta \tag{2.114}$$

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

Proposed relaxation:

$$\delta = \varepsilon\left(\max_{\boldsymbol{x}' \in V(K)}\left(\boldsymbol{u}_h^*(\boldsymbol{x}', t^i)\right) - \min_{\boldsymbol{x}' \in V(K)}\left(\boldsymbol{u}_h^*(\boldsymbol{x}', t^i)\right)\right), \tag{2.115}$$

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

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

$$\min_{\boldsymbol{x}' \in V(K)} \boldsymbol{p}_h(\boldsymbol{x}', t^i) - \delta \leq \boldsymbol{p}_h^*(\boldsymbol{x}, t^{i+1}) \leq \max_{\boldsymbol{x}' \in V(K)} \boldsymbol{p}_h(\boldsymbol{x}', t^i) + \delta \tag{2.116}$$

evaluate in terms of subcell averages.

$$\boldsymbol{p}_h^*(\boldsymbol{x}, t^{i+1}) = \boldsymbol{\mathcal{P}}\left(\boldsymbol{u}_h^*(\boldsymbol{x}, t^{i+1})\right) \tag{2.117}$$

as defined in the next section.

Important: For troubled cells that have been troubled in the previous step of the simulation we use the FVM result A(p), for newly troubled cells we use P(u).

The MUSCL-Hancock Scheme

second order in both space and time; total variation diminishing, robust, simple, details: **??**

Consists of the following steps:

1. Compute slopes:

$$\begin{aligned}\left[\hat{\boldsymbol{\delta}}_d^{K,i}\right]_{\boldsymbol{\alpha},\gamma} = \operatorname{minmod}\Bigg(&\left[\hat{\boldsymbol{p}}^{K_L,i}\right]_{\boldsymbol{\alpha}+\boldsymbol{e}_d,\gamma} - \left[\hat{\boldsymbol{p}}^{K_L,i}\right]_{\boldsymbol{\alpha},\gamma}, \\ &\left[\hat{\boldsymbol{p}}^{K_L,i}\right]_{\boldsymbol{\alpha},\gamma} - \left[\hat{\boldsymbol{p}}^{K_L,i}\right]_{\boldsymbol{\alpha}-\boldsymbol{e}_d,\gamma}\Bigg)\end{aligned} \tag{2.118}$$

for all $\boldsymbol{\alpha} \in \{0, 1, \ldots, N_S + 1\}^D := \boldsymbol{\mathcal{N}}_{\boldsymbol{\mathcal{S}}}^*$, $\gamma \in \mathcal{V}$, 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

$$\operatorname{minmod}(a, b) = \begin{cases} 0 & \text{if } ab \leq 0 \\ a & \text{if } ab > 0 \text{ and } |a| \leq |b| \\ b & \text{if } ab > 0 \text{ and } |b| < |a|. \end{cases} \tag{2.119}$$

2. Evaluate source:

$$\left[\hat{\boldsymbol{s}}^{K,i}\right]_{\boldsymbol{\alpha},\gamma} = \left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i}\right]_{\alpha}\right)\right]_{\gamma} \tag{2.120}$$

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:

$$\left[\boldsymbol{w}^{K,i}\right]_{d,e,\boldsymbol{\alpha},\gamma} = \left[\hat{\boldsymbol{u}}^{K,i}\right]_{\boldsymbol{\alpha},\gamma} + \frac{e}{2}\left[\hat{\boldsymbol{\delta}}_d^{K,i}\right]_{\boldsymbol{\alpha},\gamma} \tag{2.121}$$

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:

$$\left[\boldsymbol{w}^{K,i+\frac{1}{2}}\right]_{d,e,\boldsymbol{\alpha},\gamma} = \frac{\Delta t_i}{2} \sum_{d' \in \mathcal{D}} \sum_{e' \in \sigma} \left(e' \left[\boldsymbol{F} \left(\left[\boldsymbol{w}^{K,i} \right]_{d',e',\boldsymbol{\alpha}} \right) \right]_{\gamma,d'} / \left[\Delta \boldsymbol{x}^{L^K} \right]_{d'} \right) + \frac{\Delta t_i}{2} \left[\hat{\boldsymbol{s}}^{K,i} \right]_{\boldsymbol{\alpha},\gamma} \tag{2.122}$$

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

5. Solve Riemann problems:

$$\left[\boldsymbol{f}^{K,i}\right]_{d,\boldsymbol{\alpha},\gamma} = \left[\boldsymbol{\mathcal{G}} \left(\left[\boldsymbol{w}^{K,i+\frac{1}{2}} \right]_{d,+1,\boldsymbol{\alpha}-\boldsymbol{e}_d}, \left[\boldsymbol{w}^{K,i+\frac{1}{2}} \right]_{d,-1,\boldsymbol{\alpha}+\boldsymbol{e}_d}, \boldsymbol{e}_d \right) \right]_{\gamma} \tag{2.123}$$

6. Evolve source

$$\left[\hat{\boldsymbol{s}}^{K,i+\frac{1}{2}}\right]_{\boldsymbol{\alpha},\gamma} = \frac{1}{2} \left[\hat{\boldsymbol{s}}^{K,i} \right]_{\boldsymbol{\alpha},\gamma} + \frac{1}{2} \sum_{d' \in \mathcal{D}} \sum_{e' \in \sigma} \left(e' \left[\boldsymbol{F} \left(\left[\boldsymbol{w}^{K,i} \right]_{d',e',\boldsymbol{\alpha}} \right) \right]_{\gamma,d'} / \left[\Delta \boldsymbol{x}^{L^K} \right]_{d'} \right) \tag{2.124}$$

7. Update solution

$$\left[\boldsymbol{p}^{L^K,i+1}\right]_{\boldsymbol{\alpha},\gamma} = \left[\boldsymbol{p}^{L^K,i}\right]_{\boldsymbol{\alpha},\gamma} - \Delta t_i \sum_{d \in \mathcal{D}} \left(\left[f^{K,i} \right]_{d,\boldsymbol{\alpha}+\boldsymbol{e}_d,\gamma} - \left[f^{K,i} \right]_{d,\boldsymbol{\alpha},\gamma} / \left[\Delta \boldsymbol{x}^{L^K} \right]_{d} \right) + \Delta t_i \left[\hat{\boldsymbol{s}}^{K,i+\frac{1}{2}} \right]_{\boldsymbol{\alpha},\gamma} \tag{2.125}$$

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

Bibliography

[1] Charrier, D. E. ADER-DG on adaptive spacetrees.

[2] Dumbser, M., Enaux, C., and Toro, E. F. Finite volume schemes of very high order of accuracy for stiff hyperbolic balance laws. 3971–4001.

[3] Dumbser, M., Zanotti, O., Loubere, R., and Diot, S. A posteriori subcell limiting of the discontinuous galerkin finite element method for hyperbolic conservation laws. 47–75.

[4] John W. Eaton, David Bateman, S. H., and Wehbring, R. *GNU Octave version 4.0.0 manual: a high-level interactive language for numerical computations*.

[5] Lai, W. M., Rubin, D. H., Rubin, D., and Krempl, E. *Introduction to continuum mechanics*. Butterworth-Heinemann.

[6] Richardson, L. F. *Weather prediction by numerical process*. Cambridge University Press.

[7] Toro, E. F. *Riemann Solvers and Numerical Methods for Fluid Dynamics*. Springer Berlin Heidelberg.