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

Master's Thesis in Computational Science and Engineering

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September 2016

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

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Abstract

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Theory

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

Arbitrary High Order Derivatives Discontinuous Galerkin (ADER-DG)

2.1.1 Notation

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

2.1.2 PDE

Task: Solve the PDE

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

with initial conditions

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

and boundary conditions

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

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

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

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

have D real eigenvalues in each admissible state $(\boldsymbol{x}, t) \in \boldsymbol{\Omega} \times (0, T)$.

2.1.3 Mesh

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

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

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

Let $\{t_i\}_{i=0,1,\ldots I}$ be a partition of the time interval $(0, T)$ such that

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

where I is the number of sub intervals. We furthermore define

$$\Delta t_i = t_{i+1} - t_i, \; i \; in \left\{0, 1, \ldots, I - 1\right\}, \tag{2.8}$$

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

2.1.4 Weak formulation

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

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

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

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

which we require to hold for $v \in \{1, 2, \ldots, V\}$, $\boldsymbol{w} \in L^2(\Omega)^V$, $K \in \mathcal{K}_h$ and $i \in \{0, 1, \ldots, I - 1\}$.

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

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

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

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

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

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

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

Again we require the weak formulation to hold for all $v \in \{1, 2, \ldots V\}$, $\boldsymbol{w} \in L^2(\boldsymbol{\Omega})^V$, $K \in \mathcal{K}_h$ and $i \in \{0, 1, \ldots, I-1\}$.

2.1.5 Restriction to finite-dimensional function spaces

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

- For spatial functions we restrict ourselves to

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

- For space-time functions we restrict ourselves to

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

  for all $i \in \{0, 1, \ldots, I-1\}$.

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

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

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

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

i.e. $\tilde{\boldsymbol{u}}_h^i$ is double-valued at the interface between K and K', in order to compute the surface integral we need to introduce the numerical flux function $\boldsymbol{\mathcal{G}}(\tilde{\boldsymbol{u}}_h^{Ki}, \tilde{\boldsymbol{u}}_h^{K'i}, \boldsymbol{n})$. 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.

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

$$\int_K \left[\tilde{\boldsymbol{u}}_h^{Ki}\Big|_{t_i+\Delta t_i}\right]_v \left[\boldsymbol{w}_h^K\right]_v d\boldsymbol{x} = \int_K \left[\tilde{\boldsymbol{u}}_h^{Ki}\Big|_{t_i}\right]_v \left[\boldsymbol{w}_h^K\right]_v d\boldsymbol{x} + \\ \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{u}}_h^{Ki})\right]_{vd} \frac{\partial}{\partial x_d} \left[\boldsymbol{w}_h^K\right]_v d\boldsymbol{x}\, dt - \\ \int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{\mathcal{G}}(\tilde{\boldsymbol{u}}_h^{Ki}, \tilde{\boldsymbol{u}}_h^{K^+i}, \boldsymbol{n})\right]_v \left[\boldsymbol{w}_h^K\right]_v ds(\boldsymbol{x})\, dt + \\ \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{s}(\tilde{\boldsymbol{u}}_h^{Ki})\right]_v \left[\boldsymbol{w}_h^K\right]_v d\boldsymbol{x}\, dt. \tag{2.18}$$

Again we require eq. (2.18) to hold for all $v \in \{1, 2, \ldots, V\}$, $\boldsymbol{w}_h \in \mathbb{W}_h$, $K \in \mathcal{K}_h$ and $i \in \{0, 1, \ldots, I-1\}$.

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

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

2.1.6 Space-time predictor

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

$$\begin{aligned}
&\int_{t_i}^{t_i+\Delta t_i} \int_K \frac{\partial}{\partial t} \left[\tilde{\boldsymbol{q}}_h^{Ki}\right]_v \left[\tilde{\boldsymbol{w}}_h^{Ki}\right]_v \, d\boldsymbol{x}\, dt - \\
&\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{q}}_h^{Ki})\right]_{vd} \frac{\partial}{\partial x_d} \left[\tilde{\boldsymbol{w}}_h^{Ki}\right]_v \, d\boldsymbol{x}\, dt + \\
&\int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} \left[\boldsymbol{\mathcal{G}}\left(\tilde{\boldsymbol{q}}_h^{Ki}, \tilde{\boldsymbol{q}}_h^{K^+ i}, \boldsymbol{n}\right)\right]_v \left[\tilde{\boldsymbol{w}}_h^{Ki}\right]_v \, ds(\boldsymbol{x})\, dt = \\
&\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{s}\left(\tilde{\boldsymbol{q}}_h^{Ki}\right)\right]_v \left[\tilde{\boldsymbol{w}}_h^{Ki}\right]_v \, d\boldsymbol{x}\, dt.
\end{aligned} \tag{2.19}$$

We require eq. (2.19) to hold for all $v \in \{1, 2, \ldots, V\}$, $\tilde{\boldsymbol{w}}_h^i \in \tilde{\mathbb{W}}_h^i$, $K \in \mathcal{K}_h$ and $i \in \{0, 1, \ldots, I-1\}$.

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

$$\begin{aligned}
&\int_K \left[\tilde{\boldsymbol{q}}_h^{Ki}\Big|_{t_i+\Delta t_i}\right]_v \left[\tilde{\boldsymbol{w}}_h^{Ki}\Big|_{t_i+\Delta t_i}\right]_v d\boldsymbol{x} - \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\tilde{\boldsymbol{q}}_h^{Ki}\right]_v \frac{\partial}{\partial t} \left[\tilde{\boldsymbol{w}}_h^{Ki}\right]_v \, d\boldsymbol{x}\, dt = \\
&\int_K \left[\tilde{\boldsymbol{q}}_h^{Ki}\Big|_{t_i}\right]_v \left[\tilde{\boldsymbol{w}}_h^{Ki}\Big|_{t_i}\right]_v d\boldsymbol{x} + \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{q}}_h^{Ki})\right]_{vd} \frac{\partial}{\partial x_d} \left[\tilde{\boldsymbol{w}}_h^{Ki}\right]_v \, d\boldsymbol{x}\, dt + \\
&\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{s}\left(\tilde{\boldsymbol{q}}_h^{Ki}\right)\right]_v \left[\tilde{\boldsymbol{w}}_h^{Ki}\right]_v \, d\boldsymbol{x}\, dt,
\end{aligned} \tag{2.20}$$

which we require to hold for all $v \in \{1, 2, \ldots, V\}$, $\tilde{\boldsymbol{w}}_h^i \in \tilde{\mathbb{W}}_h^i$, $K \in \mathcal{K}_h$ and $i \in \{0, 1, \ldots, I-1\}$. Together with the initial condition

$$\tilde{\boldsymbol{q}}_h^{Ki}\Big|_{t_i} = \tilde{\boldsymbol{u}}_h^{K}\Big|_{t_i} \tag{2.21}$$

and an initial guess

$$\tilde{\boldsymbol{q}}_h^{Ki}\Big|_{t} = \tilde{\boldsymbol{u}}_h^{K}\Big|_{t_i} \;\forall t \in (t_i, t_i + \Delta t_i) \tag{2.22}$$

this relation can be used as a fixed-point iteration to find $\tilde{\boldsymbol{q}}_h^{Ki}\Big|_t$ $\forall t \in (t_i, t_i + \Delta t_i)$.

In the following two sections we will introduce mappings from space-time elements $K \times (t_i, t_i + \Delta t_i)$ to reference space-time cells and orthogonal bases for the spaces $\mathbb{W}_h$ and $\tilde{\mathbb{W}}_h^i$. We will then insert these results into eq. (2.20) and derive a fully-discrete iterative method to compute the space-time predictor $\tilde{\boldsymbol{q}}_h^{Ki}$.

2.1.7 Mappings

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

We can then introduce the following mappings:

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

$$\left[\Delta \boldsymbol{x}^K\right]_d = \max_{x \in K} [\boldsymbol{x}]_d - \min_{x \in K} [\boldsymbol{x}]_d \tag{2.23}$$

and

$$[\boldsymbol{P}_K]_d = \min_{x \in K} [\boldsymbol{x}]_d \tag{2.24}$$

for $d \in \{1, 2, \ldots, D\}$. We can then define a mapping

$$\boldsymbol{\mathcal{X}}_K : \hat{K} \to K, \boldsymbol{\xi} \mapsto \boldsymbol{\mathcal{X}}_K(\boldsymbol{\xi}) = \boldsymbol{x} \tag{2.25}$$

via the relation

$$[\boldsymbol{x}]_d = \left[\boldsymbol{\mathcal{X}}_K(\boldsymbol{\xi})\right]_d = [\boldsymbol{P}_K]_d + [\Delta \boldsymbol{x}]_d \left[\boldsymbol{\xi}\right]_d \tag{2.26}$$

for $v \in \{1, 2, \ldots, V\}$ (i.e. no summation on v) and for all $\boldsymbol{x} \in K$, $\boldsymbol{\xi} \in \hat{K}$ and $K \in \mathcal{K}_h$.

Temporal mappings: Let $(t_i, t_i + \Delta t_i), i \in \{0, 1, \ldots, I-1\}$ be an interval in global time. The mapping

$$\mathcal{T}_i : (0,1) \to (t_i, t_i + \Delta t_i), \tau \mapsto \mathcal{T}_i(\tau) = t_i + \Delta t_i \tau = t \tag{2.27}$$

maps a point in reference time $\tau \in (0,1)$ to a point in global time $t \in (t_i, t_i + \Delta t_i)$ for all $i \in \{0, 1, \ldots, I-1\}$.

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

Spatial mappings: The inverse spatial mappings

$$\boldsymbol{\mathcal{X}}_K^{-1} : K \to \hat{K}, \boldsymbol{x} \mapsto \boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x}) = \boldsymbol{\xi} \tag{2.28}$$

are defined via the relation

$$[\xi]_d = \left[\mathcal{X}_K^{-1}(\boldsymbol{x})\right]_d = \frac{1}{\left[\Delta \boldsymbol{x}^K\right]_d}\left([\boldsymbol{x}]_d - [\boldsymbol{P}_K]_d\right) \tag{2.29}$$

for $v \in \{1, 2, \ldots, V\}$ and for all $\boldsymbol{\xi} \in \hat{K}$, $\boldsymbol{x} \in K$ and $K \in \mathcal{K}_h$. The Jacobian of $\mathcal{X}_K$ is found to be

$$\left[\frac{\partial \mathcal{X}_K}{\partial \boldsymbol{\xi}}\right]_{dd'} = \frac{\partial \left[\mathcal{X}_K\right]_d}{\partial \xi_{d'}} = \left[\Delta \boldsymbol{x}^K\right]_d \delta_{dd'}, \tag{2.30}$$

where $d, d' \in \{1, 2, \ldots D\}$ (i.e. no summation on d) and for all $K \in \mathcal{K}_h$. As usual $\delta_{dd'}$ denotes the Kronecker delta defined as

$$\delta_{dd'} = \begin{cases} 0 & \text{if } d \neq d' \\ 1 & \text{if } d = d'. \end{cases} \tag{2.31}$$

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

$$J_{\mathcal{X}_K} = \| \frac{\partial \mathcal{X}_K}{\partial \boldsymbol{\xi}} \| = \prod_{d=1}^{D} \left[\Delta \boldsymbol{x}^K\right]_d, \tag{2.32}$$

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

Temporal mappings: The inverse temporal mappings are given as

$$\mathcal{T}_i^{-1} : (t_i, t_i + \Delta t_i) \to (0,1), t \mapsto \mathcal{T}_i^{-1}(t) = \frac{t - t_i}{\Delta t_i} = \tau \tag{2.33}$$

for all $\tau \in (0,1)$, $t \in (t_i, t_i + \Delta t_i)$ and $i \in \{1, 2, \ldots, I-1\}$. 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

$$\frac{d\mathcal{T}_i}{\partial \tau} = \Delta t_i = J_{\mathcal{T}_i} \tag{2.34}$$

which again is constant for all $t \in (t_i, t_i + \Delta t_i)$ for a fixed $i \in \{0, 1, \ldots, I-1\}$.

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

Lagrange interpolation

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

$$\hat{f}(\xi) = \sum_{n=0}^{N} L_n(\xi) f(\xi_n) \tag{2.35}$$

with Lagrange functions

$$L_n(\xi) = \prod_{m=0,m\neq n}^{N} \frac{\xi - \hat{\xi}_m}{\hat{\xi}_n - \hat{\xi}_m} \tag{2.36}$$

is exact, i.e.

$$f(\xi) = \hat{f}(\xi) \, \forall \xi \in (0,1). \tag{2.37}$$

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

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

$$L_n(\hat{\xi}_{n'}) = \delta_{nn'}, \tag{2.38}$$

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:

$$P_{N+1}(\xi) = \frac{1}{N+1}\left((2N+1)P_N(\xi) - nP_{N-1}(\xi)\right). \tag{2.39}$$

Let $\{\tilde{\xi}_n\}_{n\in\{0,1,\ldots,N\}}$ be the roots of the $N+1$-st Legendre polynomial L_{N+1}. Then $\{\hat{\xi}_n\}_{n\in\{0,1,\ldots,N\}}$ with

$$\hat{\xi}_n = \frac{1}{2}(\tilde{\xi}_n + 1) \tag{2.40}$$

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 $\{\hat{\omega}_n\}_{n\in\{0,1,\ldots N\}}$ Gauss-Legendre integration can be used to integrate polynomials of degree up to $2N+1$ over the integral $[0,1]$ exactly, i.e.

$$\int_0^1 f(\xi)\, d\xi = \sum_{n=0}^{N} \hat{\omega}_n f(\hat{\xi}_n) \, \forall f \in \mathbb{Q}_{2N+1}\left([0,1]\right). \tag{2.41}$$

A script on how to find the weights $\{\hat{\xi}_n\}_{n\in\{0,1,\ldots,N\}}$ can be found in appendix XXX.

1d basis functions

Let $\{\hat{\psi}_n\}_{n\in\{0,1,\ldots,N\}}$ 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.

$$\hat{\psi}_n(x) = \sum_{n'=0}^{N} \frac{x - \hat{x}_{n'}}{\hat{x}_n - \hat{x}_{n'}} \tag{2.42}$$

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

$$\left\langle \hat{\psi}_n, \hat{\psi}_m \right\rangle_{L^2\left((0,1)\right)} = \int_0^1 \hat{\psi}_n(x)\hat{\psi}_m(x)\,d\boldsymbol{x} = \sum_{n'=0}^{N} \hat{w}'_n \hat{\psi}_n(\hat{x}_{n'})\hat{\psi}_m(\hat{x}_{n'}) = \hat{w}_n\delta_{mn} \tag{2.43}$$

for all $m,n \in \{0,1,\ldots,N\}$ (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

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

$$\hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi}) = \prod_{d=1}^{D} \hat{\psi}_{[\boldsymbol{n}]_d}([\boldsymbol{\xi}]_d) = \hat{\psi}_{[\boldsymbol{n}]_d}([\boldsymbol{\xi}]_d), \tag{2.44}$$

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

$$\left[\hat{\boldsymbol{\xi}}_{\boldsymbol{n}}\right]_d = \hat{\xi}_{[\boldsymbol{n}]_d} \tag{2.45}$$

and

$$\prod_{d=1}^{D} \hat{\omega}_{[\boldsymbol{n}]_d}, \tag{2.46}$$

for all $d \in \{1,2,\ldots,D\}$ and $\boldsymbol{n} \in \{0,1,\ldots,N\}^D$, we furthermore observe that the basis is even orthogonal with respect to the L^2-scalar product, since

$$\begin{aligned} \left\langle \hat{\phi}_{\boldsymbol{n}}, \hat{\phi}_{\boldsymbol{m}} \right\rangle_{L^2(\hat{K})} &= \int_{\hat{K}} \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi})\hat{\phi}_{\boldsymbol{m}}(\boldsymbol{\xi})\,d\boldsymbol{\xi} = \\ \sum_{\boldsymbol{n}'\in\{0,1,\ldots,N\}^D} &\left(\hat{\omega}_{\boldsymbol{n}'}\hat{\phi}_{\boldsymbol{n}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{n}'})\hat{\phi}_{\boldsymbol{m}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{n}'})\right) = \hat{\omega}_{\boldsymbol{n}}\delta_{\boldsymbol{nm}} \end{aligned} \tag{2.47}$$

for all $\boldsymbol{n}, \boldsymbol{m} \in \{0, 1, \dots, N\}^D$. The natural extensions of the Kronecker delta for vector-valued indices is defined as follows:

$$\delta_{\boldsymbol{n}\boldsymbol{m}} = \prod_{d=1}^{D} \delta_{[\boldsymbol{n}]_d [\boldsymbol{m}]_d} = \delta_{[\boldsymbol{n}]_d [\boldsymbol{m}]_d}. \tag{2.48}$$

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 $\{\hat{\theta}_{\boldsymbol{n}l}\}_{\boldsymbol{n} \in \{0,1,\dots,N\}^D, l \in \{0,1,\dots,N\}}$ of $\mathbb{Q}_N(\hat{K} \times (0,1))$ on the reference space-time element $\hat{K} \times (0,1)$ as

$$\hat{\theta}_{\boldsymbol{n}l}(\boldsymbol{\xi}, \tau) = \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi}) \hat{\psi}_l(\tau), \tag{2.49}$$

which again is orthogonal, since

$$\left\langle \hat{\theta}_{\boldsymbol{n}l}, \hat{\theta}_{\boldsymbol{m}k} \right\rangle_{L^2\left(\hat{K} \times (0,1)\right)} = \int_0^1 \int_{\hat{K}} \hat{\theta}_{\boldsymbol{n}l} \hat{\theta}_{\boldsymbol{m}k} \, d\boldsymbol{\xi} \, d\tau = \hat{\omega}_{\boldsymbol{n}} \hat{\omega}_l \delta_{\boldsymbol{n}\boldsymbol{m}} \delta_{lk} \tag{2.50}$$

for all $\boldsymbol{n}, \boldsymbol{m} \in \{0, 1, \dots, N\}^D$ and $l, k \in \{0, 1, \dots, N\}$.

Vector-valued basis functions on the spatial reference element

If we define $\{\hat{\boldsymbol{\phi}}_{\boldsymbol{n}v}\}_{\boldsymbol{n} \in \{0,1,\dots,N\}^D, v \in \{1,2,\dots,V\}}$ as

$$\hat{\boldsymbol{\phi}}_{\boldsymbol{n}v} = \hat{\phi}_{\boldsymbol{n}} \boldsymbol{e}_v, \tag{2.51}$$

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

$$[\boldsymbol{e}_v]_{v'} = \delta_{vv'} \tag{2.52}$$

for all $v, v' \in \{1, 2, \dots, V\}$. Since

$$\begin{aligned} &\left\langle \hat{\boldsymbol{\phi}}_{\boldsymbol{n}v}, \hat{\boldsymbol{\phi}}_{\boldsymbol{n}'v'} \right\rangle_{L^2(\hat{K})^V} = \int_{\hat{K}} \left[\hat{\boldsymbol{\phi}}_{\boldsymbol{n}v}\right]_j \left[\hat{\boldsymbol{\phi}}_{\boldsymbol{n}'v'}\right]_j d\boldsymbol{\xi} = \\ &\left([\boldsymbol{e}_v]_j [\boldsymbol{e}_{v'}]_j\right) \int_0^1 \int_{\hat{K}} \hat{\phi}_{\boldsymbol{n}} \hat{\phi}_{\boldsymbol{n}'} \, d\boldsymbol{\xi} = \hat{\omega}_{\boldsymbol{n}} \delta_{\boldsymbol{n}\boldsymbol{n}'} \delta_{vv'} \end{aligned} \tag{2.53}$$

for all $\boldsymbol{n}, \boldsymbol{n}' \in \{0, 1, \dots, N\}^D$ and $v, v' \in \{1, 2, \dots, V\}$ 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 $\{\hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv}\}_{\boldsymbol{n} \in \{0,1,\dots,N\}^D, l \in \{0,1,\dots,N\}, v \in \{1,2,\dots,V\}}$ defined as

$$\hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv}(\boldsymbol{\xi}, \tau) = \hat{\theta}_{\boldsymbol{n}l}(\boldsymbol{\xi}, \tau) \boldsymbol{e}_v = \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi}) \hat{\psi}_l(\tau) \boldsymbol{e}_v \tag{2.54}$$

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

$$\left\langle \hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv}, \hat{\boldsymbol{\theta}}_{\boldsymbol{n}'l'v'} \right\rangle_{L^2\left(\hat{K}\times(0,1)\right)^V} = \int_0^1 \int_{\hat{K}} \left[\hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv}\right]_j \left[\hat{\boldsymbol{\theta}}_{\boldsymbol{n}'l'v'}\right]_j d\boldsymbol{\xi}\, d\tau = \hat{\omega}_{\boldsymbol{n}}\hat{\omega}_l \delta_{\boldsymbol{n}\boldsymbol{n}'}\delta_{ll'}\delta_{vv'}, \tag{2.55}$$

for all $\boldsymbol{n}, \boldsymbol{n}' \in \{0,1,\ldots,N\}^D$, $l, l' \in \{0,1,\ldots,N\}$ and $v, v' \in \{1,2,\ldots,V\}$, the set is an orthogonal basis with respect to the respective L^2-scalar product.

2.1.9 Basis functions in global coordinates

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

$$\boldsymbol{\phi}^K_{\boldsymbol{n}v}(\boldsymbol{x}) = \begin{cases} \left(\hat{\boldsymbol{\phi}}_{\boldsymbol{n}v} \circ \boldsymbol{\mathcal{X}}_K^{-1}\right)(\boldsymbol{x}) & \text{if } \boldsymbol{x} \in K \\ 0 & \text{otherwise,} \end{cases} \tag{2.56}$$

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

$$\boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv}(\boldsymbol{x}, t) = \begin{cases} \left(\hat{\boldsymbol{\theta}}_{\boldsymbol{n}lv} \circ \left(\boldsymbol{\mathcal{X}}_K^{-1}, \mathcal{T}_i^{-1}\right)\right)(\boldsymbol{x}, t) & \text{if } \boldsymbol{x} \in K \text{ and } t \in (t_i, t_i + \Delta t_i) \\ 0 & \text{otherwise} \end{cases} \tag{2.57}$$

for $\boldsymbol{n} \in \{0,1,\ldots,N\}^D$, $l \in \{0,1,\ldots,N\}$ as well as $v \in \{1,2,\ldots,V\}$ and for all $K \in \mathcal{K}_h$ and $i \in \{0,1,\ldots,I-1\}$.

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

We recall relation (2.22) for the space-time predictor. Plugging in the initial condition (2.21) yields

$$\begin{aligned} &\int_K \left[\tilde{\boldsymbol{q}}_h^{Ki}\Big|_{t_i+\Delta t_i}\right]_j \left[\tilde{\boldsymbol{w}}_h^{Ki}\Big|_{t_i+\Delta t_i}\right]_j d\boldsymbol{x} - \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\tilde{\boldsymbol{q}}_h^{Ki}\right]_j \frac{\partial}{\partial t} \left[\tilde{\boldsymbol{w}}_h^{Ki}\right]_j d\boldsymbol{x}\, dt = \\ &\int_K \left[\tilde{\boldsymbol{u}}_h^{Ki}\Big|_{t_i}\right]_j \left[\tilde{\boldsymbol{w}}_h^{Ki}\Big|_{t_i}\right]_j d\boldsymbol{x} + \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}(\tilde{\boldsymbol{q}}_h^{Ki})\right]_{jk} \frac{\partial}{\partial x_k} \left[\tilde{\boldsymbol{w}}_h^{Ki}\right]_j d\boldsymbol{x}\, dt + \\ &\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{s}\left(\tilde{\boldsymbol{q}}_h^{Ki}\right)\right]_j \left[\tilde{\boldsymbol{w}}_h^{Ki}\right]_j d\boldsymbol{x}\, dt \end{aligned} \tag{2.58}$$

which we require to hold for all $\tilde{\boldsymbol{w}}_h \in \tilde{\mathbb{W}}_h$, $K \in \mathcal{K}_h$ and $i \in \{0,1,\ldots,I-1\}$.

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

$$\tilde{\boldsymbol{q}}_h^{Ki} = \left[\hat{\boldsymbol{q}}^{Ki}\right]_{nlv} \boldsymbol{\theta}_{\boldsymbol{n}lv}^{Ki}. \tag{2.59}$$

The initial condition $\tilde{\boldsymbol{u}}_h^{Ki}\Big|_{t_i}$ can be represented as

$$\tilde{\boldsymbol{u}}_h^{Ki}\Big|_{t_i} = \left[\hat{\boldsymbol{u}}^{Ki}\right]_{nv} \boldsymbol{\phi}_{\boldsymbol{n}v}^{K}, \tag{2.60}$$

where

$$\left[\hat{\boldsymbol{u}}^{Ki}\right]_{nv} = \left[\tilde{\boldsymbol{u}}_h^{Ki}\Big|_{\left(\boldsymbol{\mathcal{X}}_K(\boldsymbol{\xi}_n), t_i\right)}\right]_v. \tag{2.61}$$

Inserting eqs. (2.59) and (2.60) into eq. (2.58) and introduction of the iteration index $r \in \{0, 1, \ldots, R\}$ leads to the following iterative scheme for the degrees of freedom of the cell-local space-time predictor:

$$\begin{aligned}
&\underbrace{\int_K \left[\left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{nlv} \boldsymbol{\theta}_{\boldsymbol{n}lv}^{Ki}\Big|_{t_i+\Delta t_i}\right]_j \left[\boldsymbol{\theta}_{\boldsymbol{\alpha}\beta\gamma}^{Ki}\Big|_{t_i+\Delta t_i}\right]_j d\boldsymbol{x}\, -}_{\text{S-I}} \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{nlv} \boldsymbol{\theta}_{\boldsymbol{n}lv}^{Ki}\right]_j \frac{\partial}{\partial t} \left[\boldsymbol{\theta}_{\boldsymbol{\alpha}\beta\gamma}^{Ki}\right]_j d\boldsymbol{x}\, dt =}_{\text{S-II}} \\
&\underbrace{\int_K \left[\left[\hat{\boldsymbol{u}}^{Ki}\right]_{nv} \boldsymbol{\phi}_{\boldsymbol{n}v}^{K}\right]_j \left[\boldsymbol{\theta}_{\boldsymbol{\alpha}\beta\gamma}^{Ki}\Big|_{t_i}\right]_j d\boldsymbol{x}\, +}_{\text{S-III}} \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{nlv} \boldsymbol{\theta}_{\boldsymbol{n}lv}^{Ki}\right)\right]_{jk} \frac{\partial}{\partial x_k} \left[\boldsymbol{\theta}_{\boldsymbol{\alpha}\beta\gamma}^{Ki}\right]_j d\boldsymbol{x}\, dt\, +}_{\text{S-IV}} \\
&\underbrace{\int_{t_i}^{t_i+\Delta t_i} \int_K \left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{nlv} \boldsymbol{\theta}_{\boldsymbol{n}lv}^{Ki}\right)\right]_j \left[\boldsymbol{\theta}_{\boldsymbol{\alpha}\beta\gamma}^{Ki}\right]_j d\boldsymbol{x}\, dt\, .}_{\text{S-V}}
\end{aligned} \tag{2.62}$$

We require this relation to hold for all $\boldsymbol{\alpha} \in \{0, 1, \ldots, N\}^D$, $\beta \in \{0, 1, \ldots, N\}$ and $\gamma \in \{1, 2, \ldots, V\}$.

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

$$\left[\hat{\boldsymbol{q}}^{K,i,0}\right]_{nvl} = \left[\hat{\boldsymbol{u}}^{Ki}\right]_{nv} \tag{2.63}$$

for all time degrees of freedom $l \in \{0, 1, \ldots, N\}$.

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

Term S-I

The first term of eq. (2.62) can be rewritten with respect to reference coordinates as follows:

$$
\begin{aligned}
&\int_K \left[\left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lw} \boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv} \Big|_{t_i+\Delta t_i} \right]_j \left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma} \right]_{t_i+\Delta t_i} d\boldsymbol{x} = \\
&\int_K \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \phi^K_{\boldsymbol{n}} \left(\psi^i_l \Big|_{t_i+\Delta t_i} \right) [\boldsymbol{e}_v]_j \, \phi^K_{\boldsymbol{\alpha}} \left(\psi^i_\beta \Big|_{t_i+\Delta t_i} \right) \left[\boldsymbol{e}_\gamma \right]_j d\boldsymbol{x} = \\
&J\boldsymbol{x}_K \int_{\hat{K}} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \hat{\phi}_{\boldsymbol{n}} \left(\hat{\psi}_l \Big|_1 \right) [\boldsymbol{e}_v]_j \, \hat{\phi}_{\boldsymbol{\alpha}} \left(\hat{\psi}_\beta \Big|_1 \right) \left[\boldsymbol{e}_\gamma \right]_j d\boldsymbol{\xi} = \\
&J\boldsymbol{x}_K \sum_{\boldsymbol{\alpha}' \in \{0,1,\ldots,N\}^D} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \hat{\phi}_{\boldsymbol{n}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \left(\hat{\psi}_l \Big|_1 \right) [\boldsymbol{e}_v]_j \, \hat{\phi}_{\boldsymbol{\alpha}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \left(\hat{\psi}_\beta \Big|_1 \right) \left[\boldsymbol{e}_\gamma \right]_j \right) = \\
&J\boldsymbol{x}_K \sum_{\boldsymbol{\alpha}' \in \{0,1,\ldots,N\}^D} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{n}lv} \delta_{\boldsymbol{n}\boldsymbol{\alpha}'} \left(\hat{\psi}_l \Big|_1 \right) \delta_{vj} \delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'} \left(\hat{\psi}_\beta \Big|_1 \right) \delta_{j\gamma} \right) = \\
&J\boldsymbol{x}_K \hat{\omega}_{\boldsymbol{\alpha}} \underbrace{\left[\hat{\psi}_\beta \Big|_1 \hat{\psi}_l \Big|_1 \right]}_{[\text{FRm?}]_{\beta l}} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{\alpha}l\gamma},
\end{aligned}
\tag{2.64}
$$

where we remember from eq. (2.32) that

$$
J\boldsymbol{x}_K = \prod_{d=1}^{D} \left[\Delta \boldsymbol{x} \right]_d . \tag{2.65}
$$

Term S-II

The second term of eq. (2.62) 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]_{nlv} \boldsymbol{\theta}^{Ki}_{nlv} \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]_{nlv} \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]_{nlv} \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 \{0,1,\ldots,N\}^D} \sum_{\beta' \in \{0,1,\ldots,N\}} \Bigg(\hat{\omega}_{\boldsymbol{\alpha}'} \hat{\omega}_{\beta'} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{nlv} \hat{\phi}_{\boldsymbol{n}}(\hat{\boldsymbol{\xi}}_{\boldsymbol{\alpha}'}) \hat{\psi}_l(\hat{\tau}_{\beta'}) \left[\boldsymbol{e}_v \right]_j \ldots \\
&\qquad \ldots \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 \{0,1,\ldots,N\}^D} \sum_{\beta' \in \{0,1,\ldots,N\}} \Bigg(\hat{\omega}_{\boldsymbol{\alpha}'} \hat{\omega}_{\beta'} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{nlv} \delta_{\boldsymbol{n}\boldsymbol{\alpha}'} \delta_{l\beta'} \delta_{vj} \ldots \\
&\qquad \ldots \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 \{0,1,\ldots,N\}} \left(\underbrace{\hat{\omega}_{\beta'} \left[\frac{\partial}{\partial \tau} \hat{\psi}_\beta(\hat{\tau}_{\beta'}) \right]}_{[Kxi?]_{\beta\beta'}} \left[\hat{\boldsymbol{q}}^{K,i,r+1} \right]_{\boldsymbol{\alpha}\beta'\gamma} \right),
\end{aligned}
\tag{2.66}
$$

where we remember from eq. (2.34) that

$$
J_{\mathcal{T}_i} = \Delta t_i, \tag{2.67}
$$

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

$$
\frac{\partial}{\partial t} \psi^i_\beta = \frac{\partial}{\partial t} \left(\hat{\psi}_\beta \circ \mathcal{T}_i^{-1} \right) = \left(\frac{\partial}{\partial \tau} \hat{\psi}_\beta \right) \left(\frac{\partial}{\partial t} \mathcal{T}_i^{-1} \right) = \frac{1}{\Delta t_i} \frac{\partial}{\partial \tau} \hat{\psi}_\beta. \tag{2.68}
$$

Term S-III

The third term of eq. (2.62) can be rewritten with respect to reference coordinates as follows:

$$\begin{aligned}
&\int_K \left[\left[\hat{\boldsymbol{u}}^{Ki} \right]_{nv} \boldsymbol{\phi}^K_{nv} \right]_j \left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma} \Big|_{t_i} \right]_j \, d\boldsymbol{x} = \\
&\int_K \left[\hat{\boldsymbol{u}}^{Ki} \right]_{nv} \phi^K_{\boldsymbol{n}} \left[\boldsymbol{e}_v \right]_j \phi^K_{\boldsymbol{\alpha}} \left(\psi^i_\beta \Big|_{t_i} \right) \left[\boldsymbol{e}_\gamma \right]_j \, d\boldsymbol{x} = \\
&J\boldsymbol{x}_K \int_{\hat{K}} \left[\hat{\boldsymbol{u}}^{Ki} \right]_{nv} \hat{\phi}_{\boldsymbol{n}} \left[\boldsymbol{e}_v \right]_j \hat{\phi}_{\boldsymbol{\alpha}} \left(\hat{\psi}_\beta \Big|_0 \right) \left[\boldsymbol{e}_\gamma \right]_j \, d\boldsymbol{\xi} = \\
&J\boldsymbol{x}_K \sum_{\boldsymbol{\alpha}' \in \{0,1,\ldots,N\}^D} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{u}}^{Ki} \right]_{nv} \hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'}) \left[\boldsymbol{e}_v \right]_j \hat{\phi}_{\boldsymbol{\alpha}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'}) \left(\hat{\psi}_\beta \Big|_0 \right) \left[\boldsymbol{e}_\gamma \right]_j \right) = \qquad (2.69) \\
&J\boldsymbol{x}_K \sum_{\boldsymbol{\alpha}' \in \{0,1,\ldots,N\}^D} \left(\hat{\omega}_{\boldsymbol{\alpha}'} \left[\hat{\boldsymbol{u}}^{Ki} \right]_{nv} \delta_{\boldsymbol{n}\boldsymbol{\alpha}'} \delta_{vj} \delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'} \left(\hat{\psi}_\beta \Big|_0 \right) \delta_{\gamma j} \right) = \\
&J\boldsymbol{x}_K \hat{\omega}_{\boldsymbol{\alpha}} \underbrace{\left[\hat{\psi}_\beta \Big|_0 \right]}_{[\mathrm{F0}]_\beta} \left[\hat{\boldsymbol{u}}^{Ki} \right]_{\boldsymbol{\alpha}\gamma} .
\end{aligned}$$

Term S-IV

The third term of eq. (2.62) can be rewritten with respect to reference coordinates as follows:

$$
\begin{aligned}
&\int_{t_i}^{t_i+\Delta t_i}\int_K \left[F\left(\left[\hat{q}^{K,i,r}\right]_{nlv}\theta^{Ki}_{nlv}\right)\right]_{jk}\frac{\partial}{\partial x_k}\left[\theta^{Ki}_{\alpha\beta\gamma}\right]_j\,dx\,dt = \\
&\int_{t_i}^{t_i+\Delta t_i}\int_K \left[F\left(\left[\hat{q}^{K,i,r}\right]_{nlv}\phi^K_n\psi^i_l e_v\right)\right]_{jk}\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\alpha]_d}([x]_d)\right)\psi^i_\beta(t)\left[e_\gamma\right]_j\cdots \\
&\cdots\left(\frac{\partial}{\partial x_k}\psi^K_{[\alpha]_k}\right)dx\,dt = \\
&J_{\mathcal{T}_i}J_{\mathcal{X}_K}\int_0^1\int_{\hat{K}}\left[F\left(\left[\hat{q}^{K,i,r}\right]_{nlv}\hat{\phi}_n\hat{\psi}_l e_v\right)\right]_{jk}\left(\prod_{d=1,d\neq k}^{D}\hat{\psi}_{[\alpha]_d}([\xi]_d)\right)\hat{\psi}_\beta(t)\left[e_\gamma\right]_j\cdots \\
&\cdots\left(\frac{1}{[\Delta x]_k}\frac{\partial}{\partial\xi_k}\hat{\psi}_{[\alpha]_k}([\xi]_k)\right)d\xi\,d\tau = \\
&J_{\mathcal{T}_i}J_{\mathcal{X}_K}\sum_{\alpha'\in\{0,1,\ldots,N\}^D}\;\sum_{\beta'\in\{0,1,\ldots,N\}}\left(\hat{\omega}_{\alpha'}\hat{\omega}_{\beta'}\left[F\left(\left[\hat{q}^{K,i,r}\right]_{nlv}\hat{\phi}_n(\hat{\xi}_{\alpha'})\hat{\psi}_l(\hat{\tau}_{\beta'})e_v\right)\right]_{jk}\cdots\right. \\
&\left.\cdots\left(\prod_{d=1,d\neq k}^{D}\hat{\psi}_{[\alpha]_d}\left(\left[\hat{\xi}_{\alpha'}\right]_d\right)\right)\hat{\psi}_\beta(\hat{\tau}_{\beta'})\left[e_\gamma\right]_j\left(\frac{1}{[\Delta x]_k}\frac{\partial}{\partial\xi_k}\hat{\psi}_{[\alpha]_k}\left(\left[\hat{\xi}_{\alpha'}\right]_k\right)\right)\right) = \\
&J_{\mathcal{T}_i}J_{\mathcal{X}_K}\sum_{\alpha'\in\{0,1,\ldots,N\}^D}\;\sum_{\beta'\in\{0,1,\ldots,N\}}\left(\hat{\omega}_{\alpha'}\hat{\omega}_{\beta'}\left[F\left(\left[\hat{q}^{K,i,r}\right]_{nlv}\delta_{n\alpha'}\delta_{l\beta'}e_v\right)\right]_{jk}\cdots\right. \\
&\left.\cdots\left(\prod_{d=1,d\neq k}^{D}\delta_{[\alpha]_d[\alpha']_d}\right)\delta_{\beta\beta'}\delta_{\gamma j}\left(\frac{1}{[\Delta x]_k}\frac{\partial}{\partial\xi_k}\hat{\psi}_{[\alpha]_k}\left(\left[\hat{\xi}_{\alpha'}\right]_k\right)\right)\right) = \\
&J_{\mathcal{T}_i}J_{\mathcal{X}_K}\hat{\omega}_\beta\sum_{k=1}^{D}\left(\frac{1}{[\Delta x]_k}\sum_{\alpha'_k\in\{0,1,\ldots,N\}}\left(\prod_{d=0,d\neq k}^{D}\hat{\omega}_{[\alpha]_d}\cdots\right.\right. \\
&\left.\left.\cdots\underbrace{\hat{\omega}_{\alpha'_k}\left(\frac{\partial}{\partial\xi_k}\hat{\psi}_{[\alpha]_k}\left(\hat{\xi}_{\alpha'_k}\right)\right)}_{[\mathrm{Kxi}]_{[\alpha]_k\alpha'_k}}\left[F\left(\left[\hat{q}^{K,i,r}\right]_{[\alpha_0,\alpha_1,\ldots,\alpha_{k-1},\alpha'_k,\alpha_{k+1},\ldots,\alpha_N]\beta v}e_v\right)\right]_{\gamma k}\right)\right),
\end{aligned}
\tag{2.70}
$$

where we used that

$$
\begin{aligned}
&\frac{\partial}{\partial x_k}\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma}(\boldsymbol{x},t) = \left(\frac{\partial}{\partial x_k}\phi^K_{\boldsymbol{\alpha}}(\boldsymbol{x})\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma = \left(\frac{\partial}{\partial x_k}\prod_{d=1}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma = \\
&\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\left(\frac{\partial}{\partial x_k}\psi^K_{[\boldsymbol{\alpha}]_k}([\boldsymbol{x}]_k)\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma = \\
&\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\left(\frac{\partial}{\partial x_k}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x})\right]_k\right)\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma = \\
&\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\left(\left(\frac{\partial}{\partial \xi_k}\hat{\psi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x})\right]_k\right)\right)\left(\frac{\partial}{\partial x_k}\left[\boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x})\right]_k\right)\right)\dots \\
&\dots\psi^i_\beta(t)\boldsymbol{e}_\gamma = \\
&\left(\prod_{d=1,d\neq k}^{D}\psi^K_{[\boldsymbol{\alpha}]_d}([\boldsymbol{x}]_d)\right)\left(\frac{1}{\left[\Delta\boldsymbol{x}^K\right]_k}\frac{\partial}{\partial \xi_k}\hat{\phi}_{[\boldsymbol{\alpha}]_k}\left(\left[\boldsymbol{\mathcal{X}}_K^{-1}(\boldsymbol{x})\right]_k\right)\right)\psi^i_\beta(t)\boldsymbol{e}_\gamma.
\end{aligned}
\tag{2.71}
$$

Term S-V

The fifth term of eq. (2.62) can be rewritten with respect to reference coordinates as follows:

$$
\begin{aligned}
&\int_{t_i}^{t_i+\Delta t_i}\int_K\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv}\boldsymbol{\theta}^{Ki}_{\boldsymbol{n}lv}\right)\right]_j\left[\boldsymbol{\theta}^{Ki}_{\boldsymbol{\alpha}\beta\gamma}\right]_j\,d\boldsymbol{x}\,dt = \\
&J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\int_0^1\int_{\hat{K}}\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv}\hat{\phi}_{\boldsymbol{n}}\hat{\psi}_l\boldsymbol{e}_v\right)\right]_j\hat{\phi}_{\boldsymbol{\alpha}}\hat{\psi}_l\left[\boldsymbol{e}_\gamma\right]_j\,d\boldsymbol{\xi}\,d\tau = \\
&J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\sum_{\boldsymbol{\alpha}'\in\{0,1,\dots,N\}^D}\sum_{\beta'\in\{0,1,\dots,N\}}\Bigg(\hat{\omega}_{\boldsymbol{\alpha}'}\hat{\omega}_{\beta'}\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv}\hat{\phi}_{\boldsymbol{n}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'})\hat{\psi}_l(\hat{\tau}_{\beta'})\boldsymbol{e}_v\right)\right]_j\dots \\
&\dots\hat{\phi}_{\boldsymbol{\alpha}}(\boldsymbol{\xi}_{\boldsymbol{\alpha}'})\hat{\psi}_\beta(\hat{\tau}_{\beta'})\left[\boldsymbol{e}_\gamma\right]_j\Bigg) = \\
&J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\sum_{\boldsymbol{\alpha}'\in\{0,1,\dots,N\}^D}\sum_{\beta'\in\{0,1,\dots,N\}}\left(\hat{\omega}_{\boldsymbol{\alpha}'}\hat{\omega}_{\beta'}\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{n}lv}\delta_{\boldsymbol{n}\boldsymbol{\alpha}'}\delta_{l\beta'}\boldsymbol{e}_v\right)\right]_j\delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'}\delta_{\beta\beta'}\delta_{\gamma j}\right) = \\
&J_{\mathcal{T}_i}J_{\boldsymbol{\mathcal{X}}_K}\hat{\omega}_{\boldsymbol{\alpha}}\hat{\omega}_\beta\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{\alpha}\beta v}\boldsymbol{e}_v\right)\right]_\gamma
\end{aligned}
\tag{2.72}
$$

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

Now collecting the results from eqs. (2.64), (2.66), (2.69), (2.70) and (2.72) and plugging them back into eq. (2.62) and division by $J_{\mathcal{X}_K}$ yields TODO: division by omega alpha

$$
\begin{aligned}
&\hat{\omega}_{\boldsymbol{\alpha}}[\mathbf{FRm}]_{\beta\beta'}\left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{\alpha}\beta'\gamma} - \\
&\hat{\omega}_{\boldsymbol{\alpha}}\left[\mathbf{Kxi}\right]_{\beta\beta'}\left[\hat{\boldsymbol{q}}^{K,i,r+1}\right]_{\boldsymbol{\alpha}\beta'\gamma} = \\
&\hat{\omega}_{\boldsymbol{\alpha}}\underbrace{\left[\hat{\psi}_{\beta}\Big|_{0}\right]}_{[\mathrm{F0}]_{\beta}}\left[\hat{\boldsymbol{u}}^{Ki}\right]_{\boldsymbol{\alpha}\gamma} + \\
&J_{\mathcal{T}_i}\hat{\omega}_{\beta}\sum_{k=1}^{D}\left(\frac{1}{[\Delta \boldsymbol{x}]_k}\sum_{\alpha'_k\in\{0,1,\ldots,N\}}\left(\prod_{d=0,d\neq k}^{D}\hat{\omega}_{[\boldsymbol{\alpha}]_d}\cdots\right.\right. \\
&\left.\left.\ldots[\mathbf{Kxi}]_{[\boldsymbol{\alpha}]_k\alpha'_k}\left[\boldsymbol{F}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{[\alpha_0,\alpha_1,\ldots,\alpha_{k-1},\alpha'_k,\alpha_{k+1},\ldots,\alpha_N]\beta v}\boldsymbol{e}_v\right)\right]_{\gamma k}\right)\right) + \\
&J_{\mathcal{T}_i}\hat{\omega}_{\boldsymbol{\alpha}}\hat{\omega}_{\beta}\left[\boldsymbol{s}\left(\left[\hat{\boldsymbol{q}}^{K,i,r}\right]_{\boldsymbol{\alpha}\beta v}\boldsymbol{e}_v\right)\right]_{\gamma},
\end{aligned}
\tag{2.73}
$$

which has to hold for all $\boldsymbol{\alpha} \in \{0,1,\ldots,N\}^D$, $\beta \in \{0,1,\ldots,N\}$ and $\gamma \in \{1,2,\ldots,V\}$.

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

TODO: Add appendix with code that computes all matrices

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

Now that we have developed a method to compute the space-time predictor, we can go back to the original one-step, cell-local update scheme given in eq. (2.18).

Discretization

Plug in

Treat term-by-term

Final result

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