



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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Chapter 1

Introduction

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

Chapter 2

Theory

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

Arbitrary High Order Derivatives Discontinuous Galerkin (ADER-DG)

2.1.1 Notation

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

2.1.2 PDE

Task: Solve the PDE

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

with initial conditions

$$[u(x, 0)]_v = [u_0(x)]_v \quad \forall x \in \Omega, \quad (2.2)$$

and boundary conditions

$$[u(x, t)]_v = [u_B(x, t)]_v \quad \forall x \in \partial\Omega, t \in (0, T), \quad (2.3)$$

for all $v \in \{1, 2, \dots, V\}$, where V is the number of quantities involved in the system, $\Omega \subset \mathbb{R}^D$ is the spatial domain, D the number of space dimensions, and $(0, T)$ a time interval. The function $F : \mathbb{R}^V \rightarrow \mathbb{R}^{V \times D}, u \mapsto F(u) = [f_1(u), f_2(u), \dots, f_D(u)]$ is called the flux function.

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

$$[A_d]_{ij} = \frac{\partial [f_d]_i}{\partial x_j}, \quad (2.4)$$

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

2.1.3 Mesh

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

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

$$\bigcup_{K \in \mathcal{K}_h} K = \Omega. \quad (2.6)$$

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

$$0 = t_0 < t_1 < \dots < t_I = T, \quad (2.7)$$

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

$$\Delta t_i = t_{i+1} - t_i, \quad i \text{ in } \{0, 1, \dots, I-1\}, \quad (2.8)$$

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

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

Let $\mathbf{w} \in L^2(\Omega)^V$ 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

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

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

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

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

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

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

where $\mathbf{n} \in \mathbb{R}^D$ is the unit-length, outward-pointing normal vector at a point \mathbf{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):

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

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

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 $\mathbf{Q}_N(K)^V$ and $\mathbf{Q}_N(K \times (t_i, t_i + \Delta t_i))^V$ 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

$$\mathbf{W}_h = \left\{ w_h \in L^2(\Omega)^V : w_h|_K := w_h^K \in \mathbf{Q}_N(K)^V \forall K \in \mathcal{K}_h \right\}. \quad (2.14)$$

- For space-time functions we restrict ourselves to

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

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

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

$$\begin{aligned} & \int_{t_i}^{t_i+\Delta t_i} \int_K \frac{\partial}{\partial t} [\tilde{u}_h^{Ki}]_v [w_h^K]_v dx dt - \int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} [F(\tilde{u}_h^{Ki})]_{vd} \frac{\partial}{\partial x_d} [w_h^K]_v dx dt + \\ & \int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} [\mathcal{G}(\tilde{u}_h^{Ki}, \tilde{u}_h^{K+i}, n)]_v [w_h^K]_v ds(x) dt = \\ & \int_{t_i}^{t_i+\Delta t_i} \int_K [s(\tilde{u}_h^{Ki})]_v [w_h^K]_v dx dt, \end{aligned} \quad (2.16)$$

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

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

i.e. \tilde{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 $\mathcal{G}(\tilde{u}_h^{Ki}, \tilde{u}_h^{K'i}, n)$. The numerical flux at a position $x \in K \cap K'$ 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 w_h is constant in time yields the following one-step update scheme for the cell-local time-discrete solution \tilde{u}_h^{Ki} :

$$\begin{aligned} \int_K [\tilde{u}_h^{Ki}]_{t_i+\Delta t_i} [w_h^K]_v dx &= \int_K [\tilde{u}_h^{Ki}]_{t_i} [w_h^K]_v dx + \\ & \int_{t_i}^{t_i+\Delta t_i} \int_K [F(\tilde{u}_h^{Ki})]_{vd} \frac{\partial}{\partial x_d} [w_h^K]_v dx dt - \\ & \int_{t_i}^{t_i+\Delta t_i} \int_{\partial K} [\mathcal{G}(\tilde{u}_h^{Ki}, \tilde{u}_h^{K+i}, n)]_v [w_h^K]_v ds(x) dt + \\ & \int_{t_i}^{t_i+\Delta t_i} \int_K [s(\tilde{u}_h^{Ki})]_v [w_h^K]_v dx dt. \end{aligned} \quad (2.18)$$

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

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

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

2.1.6 Space-time predictor

To derive a procedure to compute the space-time predictor $\tilde{\mathbf{q}}_h^i \in \tilde{\mathbb{W}}_h^i$ we again start from the original PDE (2.1), but this time we do not use a spatial test function $\mathbf{w}_h \in \mathbb{W}_h$, but a space-time test function $\tilde{\mathbf{w}}_h^i \in \tilde{\mathbb{W}}_h^i$. If we furthermore replace the solution \mathbf{u} by the space-time predictor $\tilde{\mathbf{q}}_h^i \in \tilde{\mathbb{W}}_h^i$, 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:

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

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

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

$$\begin{aligned} & \int_K [\tilde{\mathbf{q}}_h^{Ki}]_{t_i+\Delta t_i} [\tilde{\mathbf{w}}_h^{Ki}]_{t_i+\Delta t_i} dx - \int_{t_i}^{t_i+\Delta t_i} \int_K [\tilde{\mathbf{q}}_h^{Ki}]_v \frac{\partial}{\partial t} [\tilde{\mathbf{w}}_h^{Ki}]_v dx dt = \\ & \int_K [\tilde{\mathbf{q}}_h^{Ki}]_{t_i} [\tilde{\mathbf{w}}_h^{Ki}]_{t_i} dx + \int_{t_i}^{t_i+\Delta t_i} \int_K [F(\tilde{\mathbf{q}}_h^{Ki})]_{vd} \frac{\partial}{\partial x_d} [\tilde{\mathbf{w}}_h^{Ki}]_v dx dt + \\ & \int_{t_i}^{t_i+\Delta t_i} \int_K [s(\tilde{\mathbf{q}}_h^{Ki})]_v [\tilde{\mathbf{w}}_h^{Ki}]_v dx dt, \end{aligned} \quad (2.20)$$

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

$$\tilde{\mathbf{q}}_h^{Ki} \Big|_{t_i} = \tilde{\mathbf{u}}_h^K \Big|_{t_i} \quad (2.21)$$

and an initial guess

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

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

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{q}_h^{Ki} .

2.1.7 Mappings

Let $\hat{K} = (0, 1)^D$ be the spatial reference element and $\xi \in \hat{K}$ 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 Δx^K and “lower-left corner” P_K , more precisely that is

$$[\Delta x^K]_d = \max_{x \in K} [x]_d - \min_{x \in K} [x]_d \quad (2.23)$$

and

$$[P_K]_d = \min_{x \in K} [x]_d \quad (2.24)$$

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

$$\mathcal{X}_K : \hat{K} \rightarrow K, \xi \mapsto \mathcal{X}_K(\xi) = x \quad (2.25)$$

via the relation

$$[x]_d = [\mathcal{X}_K(\xi)]_d = [P_K]_d + [\Delta x^K]_d [\xi]_d \quad (2.26)$$

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

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

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

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 $i \in \{0, 1, \dots, I - 1\}$.

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

Spatial mappings: The inverse spatial mappings

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

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are defined via the relation

$$[\xi]_d = [\mathcal{X}_K^{-1}(x)]_d = \frac{1}{[\Delta x^K]_d} ([x]_d - [P_K]_d) \quad (2.29)$$

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

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

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

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

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

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

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

Temporal mappings: The inverse temporal mappings are given as

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

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

$$\frac{d\mathcal{T}_i}{d\tau} = \Delta t_i = J_{\mathcal{T}_i} \quad (2.34)$$

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

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 $\{\hat{\xi}_n\}_{n \in \{0, 1, \dots, N\}}$ be a set of distinct nodes in $(0, 1)$. The the Lagrange interpolation of f ,

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

with Lagrange functions

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

is exact, i.e.

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

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

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

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

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

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

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

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

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

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

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

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1d basis functions

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

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

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

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

for all $m, n \in \{0, 1, \dots, N\}$ (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 $\{\hat{\phi}_n\}_{n \in \{0,1,\dots,N\}^D}$ on $\hat{K} = [0, 1]^D$ as

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

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

$$[\hat{\xi}_n]_d = \hat{\xi}_{[n]_d} \quad (2.45)$$

and

$$\prod_{d=1}^D \hat{\omega}_{[n]_d}, \quad (2.46)$$

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

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

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

$$\delta_{nm} = \prod_{d=1}^D \delta_{[n]_d [m]_d} = \delta_{[n]_d [m]_d}. \quad (2.48)$$

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

$$\hat{\theta}_{nl}(\boldsymbol{\xi}, \tau) = \hat{\phi}_n(\boldsymbol{\xi}) \hat{\psi}_l(\tau), \quad (2.49)$$

which again is orthogonal, since

$$\langle \hat{\theta}_{nl}, \hat{\theta}_{mk} \rangle_{L^2(\hat{K} \times (0,1))} = \int_0^1 \int_{\hat{K}} \hat{\theta}_{nl} \hat{\theta}_{mk} d\boldsymbol{\xi} d\tau = \hat{\omega}_n \hat{\omega}_l \delta_{nm} \delta_{lk} \quad (2.50)$$

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

Vector-valued basis functions on the spatial reference element

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

$$\hat{\phi}_{nv} = \hat{\phi}_n \mathbf{e}_v, \quad (2.51)$$

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

$$[\mathbf{e}_v]_{v'} = \delta_{vv'} \quad (2.52)$$

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

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

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

$$\hat{\theta}_{nlv}(\boldsymbol{\xi}, \tau) = \hat{\theta}_{nl}(\boldsymbol{\xi}, \tau) \mathbf{e}_v = \hat{\phi}_n(\boldsymbol{\xi}) \hat{\psi}_l(\tau) \mathbf{e}_v \quad (2.54)$$

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

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

for all $\mathbf{n}, \mathbf{n}' \in \{0, 1, \dots, N\}^D$, $l, l' \in \{0, 1, \dots, N\}$ and $v, v' \in \{1, 2, \dots, V\}$, 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

$$\phi_{nv}^K(\mathbf{x}) = \begin{cases} \left(\hat{\phi}_{nv} \circ \mathcal{X}_K^{-1} \right)(\mathbf{x}) & \text{if } \mathbf{x} \in K \\ 0 & \text{otherwise,} \end{cases} \quad (2.56)$$

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

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

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

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

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

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

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

$$\tilde{\mathbf{q}}_h^{Ki} = \left[\hat{\mathbf{q}}^{Ki} \right]_{nlv} \boldsymbol{\theta}_{nlv}^{Ki}. \quad (2.59)$$

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

$$\tilde{\mathbf{u}}_h^{Ki}|_{t_i} = \left[\hat{\mathbf{u}}^{Ki} \right]_{nv} \boldsymbol{\phi}_{nv}^K, \quad (2.60)$$

where

$$\left[\hat{\mathbf{u}}^{Ki} \right]_{nv} = \left[\tilde{\mathbf{u}}_h^{Ki} \Big|_{(\mathbf{x}_K(\xi_n), t_i)} \right]_v. \quad (2.61)$$

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

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

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

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

$$\left[\hat{\mathbf{q}}^{K,i,0} \right]_{nlv} = \left[\hat{\mathbf{u}}^{Ki} \right]_{nv} \quad (2.63)$$

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

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 $\hat{q}^{K,i,r+1}$ that holds for all $K \in \mathcal{K}_h$.

Term 1

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

$$\begin{aligned}
 & \int_K \left[\left[\hat{q}^{K,i,r+1} \right]_{nlv} \theta_{nlv}^{Ki} \Big|_{t_i+\Delta t_i} \right]_j \left[\theta_{\alpha\beta\gamma}^{Ki} \right]_{t_i+\Delta t_i} dx = \\
 & \int_K \left[\hat{q}^{K,i,r+1} \right]_{nlv} \phi_n^K \left(\psi_l^i \Big|_{t_i+\Delta t_i} \right) [e_v]_j \phi_\alpha^K \left(\psi_\beta^i \Big|_{t_i+\Delta t_i} \right) [e_\gamma]_j dx = \\
 & J\mathcal{X}_K \int_{\hat{K}} \left[\hat{q}^{K,i,r+1} \right]_{nlv} \hat{\phi}_n \left(\hat{\psi}_l \Big|_1 \right) [e_v]_j \hat{\phi}_\alpha \left(\hat{\psi}_\beta \Big|_1 \right) [e_\gamma]_j d\hat{\xi} = \\
 & J\mathcal{X}_K \sum_{\alpha' \in \{0,1,\dots,N\}^D} \left(\hat{\omega}_{\alpha'} \left[\hat{q}^{K,i,r+1} \right]_{nlv} \hat{\phi}_n(\hat{\xi}_{\alpha'}) \left(\hat{\psi}_l \Big|_1 \right) [e_v]_j \hat{\phi}_\alpha(\hat{\xi}_{\alpha'}) \left(\hat{\psi}_\beta \Big|_1 \right) [e_\gamma]_j \right) = \\
 & J\mathcal{X}_K \sum_{\alpha' \in \{0,1,\dots,N\}^D} \left(\hat{\omega}_{\alpha'} \left[\hat{q}^{K,i,r+1} \right]_{nlv} \delta_{n\alpha'} \left(\hat{\psi}_l \Big|_1 \right) \delta_{vj} \delta_{\alpha\alpha'} \left(\hat{\psi}_\beta \Big|_1 \right) \delta_{j\gamma} \right) = \\
 & J\mathcal{X}_K \underbrace{\hat{\omega}_\alpha \left[\hat{\psi}_\beta \Big|_1 \hat{\psi}_l \Big|_1 \right]}_{[\text{FRm?}]_{\beta l}} \left[\hat{q}^{K,i,r+1} \right]_{\alpha l \gamma},
 \end{aligned} \tag{2.64}$$

where we remember from eq. (2.32) that

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

Term 2

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[\hat{\mathbf{q}}^{K,i,r+1} \right]_{nlv} \boldsymbol{\theta}_{nlv}^{Ki} \left[\frac{\partial}{\partial t} \left[\boldsymbol{\theta}_{\alpha\beta\gamma}^{Ki} \right]_j \right] dx dt = \\
 & \int_{t_i}^{t_i+\Delta t_i} \int_K \left[\hat{\mathbf{q}}^{K,i,r+1} \right]_{nlv} \phi_n^K \psi_l^i [e_v]_j \phi_\alpha^K \left(\frac{\partial}{\partial t} \psi_\beta^i \right) [e_\gamma]_j dx dt = \\
 & J_{\mathcal{T}_i} J_{\mathcal{X}_K} \int_0^1 \int_{\hat{K}} \left[\hat{\mathbf{q}}^{K,i,r+1} \right]_{nlv} \hat{\phi}_n \hat{\psi}_l [e_v]_j \hat{\phi}_\alpha \left(\frac{1}{\Delta t_i} \frac{\partial}{\partial \tau} \hat{\psi}_\beta \right) [e_\gamma]_j d\xi d\tau = \\
 & J_{\mathcal{T}_i} J_{\mathcal{X}_K} \sum_{\alpha' \in \{0,1,\dots,N\}^D} \sum_{\beta' \in \{0,1,\dots,N\}} \left(\hat{\omega}_{\alpha'} \hat{\omega}_{\beta'} \left[\hat{\mathbf{q}}^{K,i,r+1} \right]_{nlv} \hat{\phi}_n(\hat{\xi}_{\alpha'}) \hat{\psi}_l(\hat{\tau}_{\beta'}) [e_v]_j \dots \right. \\
 & \quad \left. \dots \hat{\phi}_\alpha(\hat{\xi}_{\alpha'}) \left(\frac{\partial}{\partial \tau} \hat{\psi}_\beta(\hat{\tau}_{\beta'}) \right) [e_\gamma]_j \right) = \\
 & J_{\mathcal{T}_i} J_{\mathcal{X}_K} \sum_{\alpha' \in \{0,1,\dots,N\}^D} \sum_{\beta' \in \{0,1,\dots,N\}} \left(\hat{\omega}_{\alpha'} \hat{\omega}_{\beta'} \left[\hat{\mathbf{q}}^{K,i,r+1} \right]_{nlv} \delta_{n\alpha'} \delta_{l\beta'} \delta_{vj} \dots \right. \\
 & \quad \left. \dots \delta_{\alpha\alpha'} \left(\frac{1}{\Delta t_i} \frac{\partial}{\partial \tau} \hat{\psi}_\beta(\hat{\tau}_{\beta'}) \right) \delta_{\gamma j} \right) = \\
 & J_{\mathcal{T}_i} J_{\mathcal{X}_K} \hat{\omega}_\alpha \frac{1}{\Delta t_i} \sum_{\beta' \in \{0,1,\dots,N\}} \left(\underbrace{\hat{\omega}_{\beta'} \left[\frac{\partial}{\partial \tau} \hat{\psi}_\beta(\hat{\tau}_{\beta'}) \right]}_{[Kxi?]_{\beta\beta'}} \left[\hat{\mathbf{q}}^{K,i,r+1} \right]_{\alpha\beta'\gamma} \right), \tag{2.66}
 \end{aligned}$$

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. (2.66) cancel. In the derivation we made use of the fact that due to the chain rule

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

Term 3

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

$$\begin{aligned}
 & \int_K \left[\left[\hat{\mathbf{u}}^{Ki} \right]_{nv} \boldsymbol{\phi}_{nv}^K \right]_j \left[\boldsymbol{\theta}_{\alpha\beta\gamma}^{Ki} \Big|_{t_i} \right]_j d\mathbf{x} = \\
 & \int_K \left[\left[\hat{\mathbf{u}}^{Ki} \right]_{nv} \boldsymbol{\phi}_n^K [\mathbf{e}_v]_j \boldsymbol{\phi}_\alpha^K \left(\psi_\beta^i \Big|_{t_i} \right) \right]_j [\mathbf{e}_\gamma]_j d\mathbf{x} = \\
 & J_{\mathcal{X}_K} \int_{\hat{K}} \left[\left[\hat{\mathbf{u}}^{Ki} \right]_{nv} \hat{\boldsymbol{\phi}}_n [\mathbf{e}_v]_j \hat{\boldsymbol{\phi}}_\alpha \left(\hat{\psi}_\beta \Big|_0 \right) \right]_j [\mathbf{e}_\gamma]_j d\boldsymbol{\xi} = \\
 & J_{\mathcal{X}_K} \sum_{\alpha' \in \{0,1,\dots,N\}^D} \left(\hat{\omega}_{\alpha'} \left[\left[\hat{\mathbf{u}}^{Ki} \right]_{nv} \hat{\boldsymbol{\phi}}_n(\boldsymbol{\xi}_{\alpha'}) [\mathbf{e}_v]_j \hat{\boldsymbol{\phi}}_\alpha(\boldsymbol{\xi}_{\alpha'}) \left(\hat{\psi}_\beta \Big|_0 \right) \right]_j [\mathbf{e}_\gamma]_j \right) = \quad (2.69) \\
 & J_{\mathcal{X}_K} \sum_{\alpha' \in \{0,1,\dots,N\}^D} \left(\hat{\omega}_{\alpha'} \left[\left[\hat{\mathbf{u}}^{Ki} \right]_{nv} \delta_{n\alpha'} \delta_{vj} \delta_{\alpha\alpha'} \left(\hat{\psi}_\beta \Big|_0 \right) \delta_{\gamma j} \right] \right) = \\
 & J_{\mathcal{X}_K} \underbrace{\hat{\omega}_\alpha \left[\hat{\psi}_\beta \Big|_0 \right]}_{[\mathbf{F0}]_\beta} \left[\left[\hat{\mathbf{u}}^{Ki} \right]_{\alpha\gamma} \right].
 \end{aligned}$$

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 $\Delta x \rightarrow$ Error for polynomials (convergence tables)

Chapter 5

Conclusion and Outlook

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

Chapter 6

Acknowledgment
