



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

Master's Thesis in Computational Science and Engineering

**Fabian Gura**

Department of Informatics  
Technische Universität München

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

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# Introduction

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



## Chapter 2

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# Theory

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### 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.

## 2. THEORY

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

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

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

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  $\Omega$ , 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  $v \in \{1, 2, \dots, V\}$ ,  $\mathbf{w} \in L^2(\Omega)^V$ ,  $K \in \mathcal{T}_h$  and  $i \in \{0, 1, \dots, I-1\}$ .

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

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

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

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

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

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  $\partial K$ .

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

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

Again we require the weak formulation to hold for all  $v \in \{1, 2, \dots, V\}$ ,  $\mathbf{w} \in L^2(\Omega)^V$ ,  $K \in \mathcal{T}_h$  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

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

- For space-time functions we restrict ourselves to

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

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

## 2. THEORY

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  $w_h \in \mathbb{W}_h$ ,  $K \in \mathcal{T}_h$  and  $i \in \{0, 1, \dots, I-1\}$ . Since for a cell  $K \in \mathcal{T}_h$  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  $v \in \{1, 2, \dots, V\}$ ,  $w_h \in \mathbb{W}_h$ ,  $K \in \mathcal{T}_h$  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:

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

We require eq. (2.19) to hold for all  $v \in \{1, 2, \dots, V\}$ ,  $\tilde{\mathbf{w}}_h^i \in \tilde{\mathbb{W}}_h^i$ ,  $K \in \mathcal{T}_h$  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  $K \in \mathcal{T}_h$  allows us to drop the third term. Together with integration by parts in time of the first term this yields

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

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

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

and an initial guess

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

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

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  $W_h$  and  $\tilde{W}_h^i$ . 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  $K \in \mathcal{T}_h$  be a cell in global coordinates with extent  $\Delta x^K$  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

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

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

**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

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



are defined via the relation

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

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

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

where  $d, d' \in \{1, 2, \dots, D\}$  (i.e. no summation on  $d$ ) and for all  $K \in \mathcal{T}_h$ . 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  $K \in \mathcal{T}_h$  then simply is

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

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

## 2.2 Profiling and Energy-aware Computing



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## **A profiling infrastructure for ExaHyPE**

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- General architecture
- Architecture profiling
- Functionality



## Chapter 4

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# Preliminary profiling results, case studies

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- 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

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# Conclusion and Outlook

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





## Chapter 6

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# Acknowledgment

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