



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

Master's Thesis in Computational Science and Engineering

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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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## Chapter 2

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# Theory

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Equation:

$$\mathbf{Q}_t + \nabla \cdot \mathbf{F}(\mathbf{Q}) = 0, \quad \mathbf{x} \in \Omega, \quad t \in \mathbb{R}_0^+, \quad (2.1)$$

where  $\mathbf{Q} \in \Omega_Q \subset \mathbb{R}^\nu$  is the state vector of  $\nu$  conserved quantities, and  $\mathbf{F}(\mathbf{Q}) = (f, g, h)$  is a non-linear flux tensor that depends on the state  $\mathbf{Q}$ .  $\Omega$  denotes the computational domain in  $d$  space dimensions where  $\Omega_Q$  is the space of physically admissible state, also called state space or phase-space.

Initial conditions:

$$\mathbf{Q}(\mathbf{x}, 0) = \mathbf{Q}_0(\mathbf{x}) \quad \forall \mathbf{x} \in \Omega \quad (2.2)$$

Dirichlet boundary conditions:

$$\mathbf{Q}(\mathbf{x}, t) = \mathbf{Q}_B(\mathbf{x}, t) \quad \forall \mathbf{x} \in \partial\Omega, \quad t \in \mathbb{R}_0^+ \quad (2.3)$$

Space discretization main grid  $\mathcal{T}_\Omega = \{T_i, i = 1, \dots, N_E\}$  is a partition of the domain  $\Omega$ , i.e.

$$\bigcup_{i=1}^{N_E} T_i = \Omega \quad \text{and} \quad (2.4)$$

$$T \cap U = \emptyset \quad \forall T, U \in \mathcal{T}_\Omega, T \neq U \quad (2.5)$$

Cell volume:

$$|T_i| = \int_{T_i} d\mathbf{x} \quad (2.6)$$

At the beginning of each time-step the state vector  $\mathbf{Q}$  is represented within each cell  $T_i$  of the main grid by piecewise polynomials of maximum degree  $N \geq 0$  and is denoted by

$$\mathbf{u}_h(\mathbf{x}, t) = \sum_l \Phi_l(\mathbf{x}) \hat{\mathbf{u}}_l^n = \Phi_l(\mathbf{x}) \hat{\mathbf{u}}_l^n \quad (2.7)$$

## 2. THEORY

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Transformation to space-time reference coordinate system  $(\xi, t)$ :

$$t = t + \tau \Delta t \leftrightarrow \tau = \frac{t - t^n}{t^{n+1} - t^n} \quad (2.8)$$

$$\mathbf{x} = \mathbf{x}_l + (\mathbb{I}\xi)\Delta\mathbf{x} \leftrightarrow \xi = \xi = (\mathbb{I}\Delta\mathbf{x})^{-1}(\mathbf{x} - \mathbf{x}_l), \quad (2.9)$$

where  $\Delta t = t^{n+1} - t^n$  and  $\Delta\mathbf{x} = \mathbf{x}_r - \mathbf{x}_l$  and  $\mathbf{x}_l$  and  $\mathbf{x}_r$  are the lower left and the upper right corner of the cell, respectively. More formal that is

$$(\mathbf{x}_l)_i = \min_{\mathbf{x} \in T_i} \{(\mathbf{x})_i\}, \quad i = 1, \dots, d \quad (2.10)$$

$$(\mathbf{x}_r)_i = \max_{\mathbf{x} \in T_i} \{(\mathbf{x})_i\}, \quad i = 1, \dots, d. \quad (2.11)$$

The respective transformation matrices are given as follows:

$$(\mathbb{I}\Delta\mathbf{x})_{ij} = \begin{bmatrix} (\Delta\mathbf{x})_1 & 0 & \dots & 0 \\ 0 & (\Delta\mathbf{x})_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & (\Delta\mathbf{x})_d \end{bmatrix} \quad (2.12)$$

$$(\mathbb{I}\Delta\mathbf{x})_{ij}^{-1} = \begin{bmatrix} 1/(\Delta\mathbf{x})_1 & 0 & \dots & 0 \\ 0 & 1/(\Delta\mathbf{x})_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1/(\Delta\mathbf{x})_d \end{bmatrix}. \quad (2.13)$$

Now one has for the time derivative

$$\frac{\partial Q}{\partial t} = \frac{\partial Q}{\partial \tau} \frac{\partial \tau}{\partial t} = \frac{\partial Q}{\partial \tau} \frac{1}{t^{n+1} - t^n} = \frac{1}{\Delta t} Q_t, \quad (2.14)$$

and for the spatial derivative (Note:  $\mathbf{x} = [x \ y \ z]^T$  and  $\xi = [\xi \ \eta \ \zeta]^T$ )

$$\nabla_{\mathbf{x}} \cdot F(Q) = \frac{\partial f}{\partial x}(Q) + \frac{\partial g}{\partial y}(Q) + \frac{\partial h}{\partial z}(Q), \quad (2.15)$$

furthermore

$$\begin{aligned} \frac{\partial f}{\partial x} &= \frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial f}{\partial \eta} \frac{\partial \eta}{\partial x} + \frac{\partial f}{\partial \zeta} \frac{\partial \zeta}{\partial x} \\ \frac{\partial g}{\partial y} &= \frac{\partial g}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial g}{\partial \eta} \frac{\partial \eta}{\partial y} + \frac{\partial g}{\partial \zeta} \frac{\partial \zeta}{\partial y} \\ \frac{\partial h}{\partial z} &= \frac{\partial h}{\partial \xi} \frac{\partial \xi}{\partial z} + \frac{\partial h}{\partial \eta} \frac{\partial \eta}{\partial z} + \frac{\partial h}{\partial \zeta} \frac{\partial \zeta}{\partial z} \end{aligned} \quad (2.16)$$

so that

$$\begin{aligned}
\nabla_x \cdot \mathbf{F} &= \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} + \frac{\partial h}{\partial z} \\
&= \left( \frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial f}{\partial \eta} \frac{\partial \eta}{\partial x} + \frac{\partial f}{\partial \zeta} \frac{\partial \zeta}{\partial x} \right) + \\
&\quad \left( \frac{\partial g}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial g}{\partial \eta} \frac{\partial \eta}{\partial y} + \frac{\partial g}{\partial \zeta} \frac{\partial \zeta}{\partial y} \right) + \\
&\quad \left( \frac{\partial h}{\partial \xi} \frac{\partial \xi}{\partial z} + \frac{\partial h}{\partial \eta} \frac{\partial \eta}{\partial z} + \frac{\partial h}{\partial \zeta} \frac{\partial \zeta}{\partial z} \right) \\
&= \left( \frac{\partial \xi}{\partial x} \frac{\partial f}{\partial \xi} + \frac{\partial \xi}{\partial y} \frac{\partial g}{\partial \xi} + \frac{\partial \xi}{\partial z} \frac{\partial h}{\partial \xi} \right) \\
&\quad \left( \frac{\partial \eta}{\partial x} \frac{\partial f}{\partial \eta} + \frac{\partial \eta}{\partial y} \frac{\partial g}{\partial \eta} + \frac{\partial \eta}{\partial z} \frac{\partial h}{\partial \eta} \right) + \\
&\quad \left( \frac{\partial \zeta}{\partial x} \frac{\partial f}{\partial \zeta} + \frac{\partial \zeta}{\partial y} \frac{\partial g}{\partial \zeta} + \frac{\partial \zeta}{\partial z} \frac{\partial h}{\partial \zeta} \right) \\
&= \nabla_\xi \cdot \left( [f \quad g \quad h] \begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} & \frac{\partial \xi}{\partial z} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} & \frac{\partial \eta}{\partial z} \\ \frac{\partial \zeta}{\partial x} & \frac{\partial \zeta}{\partial y} & \frac{\partial \zeta}{\partial z} \end{bmatrix}^T \right) \\
&= \nabla_\xi \cdot \left( \mathbf{F} \left( \frac{\partial \xi}{\partial x} \right)^T \right),
\end{aligned} \tag{2.17}$$

where

$$\left( \frac{\partial \xi}{\partial x} \right)_{ij} = \frac{\partial \xi_i}{\partial x_j}. \tag{2.18}$$

The PDE can then be rewritten with respect to the reference coordinates as follows:

$$\frac{\partial Q}{\partial \tau} + \nabla_\xi F^*(Q) = 0, \tag{2.19}$$

where the modified flux is defined as

$$F^* := \Delta t F(Q) \left( \frac{\partial \xi}{\partial x} \right)^T. \tag{2.20}$$

To simplify notation, let us define the following two operators:

$$\langle f, g \rangle = \int_0^1 \int_{T_E} (f(\xi, \tau) \cdot g(\xi, \tau)) d\xi d\tau \tag{2.21}$$

$$[f, g] = \int_{T_E} (f(\xi, \tau) \cdot g(\xi, \tau)) d\xi \tag{2.22}$$

## 2. THEORY

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Lagrange basis function 1D:

$$L_i(\xi) = \prod_{j \neq i} \frac{\xi - \xi_j}{\xi_i - \xi_j}, \quad (2.23)$$

where  $\xi_j$  are the Gauss-Legendre points mapped to the interval  $[0, 1]$ .

Stiffness matrix:

$$K_{ij} = \int_{T_E} \Phi_{i,\xi} \Phi_j d\xi, \quad (2.24)$$

where  $T_E$  is the reference element  $[0; 1]^d$  and  $d$  is the dimensionality of the setup.

Mass matrix:

$$M_{ij} = \int_{T_E} \Phi_i \Phi_j d\xi \quad (2.25)$$

## Chapter 3

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# Conclusion and Outlook

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## Chapter 4

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# Acknowledgment

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