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
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Abstract

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Theory

Equation:

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

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

Initial conditions:

$$Q(x, 0) = Q_0(x) \quad \forall x \in \Omega \tag{2.2}$$

Dirichlet boundary conditions:

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

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

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

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

Cell volume:

$$|T_i| = \int_{T_i} dx \tag{2.6}$$

At the beginning of each time-step the state vector 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

$$u_h(x, t) = \sum_l \Phi_l(x)\hat{u}_l^n = \Phi_l(x)\hat{u}_l^n \tag{2.7}$$

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

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

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

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

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

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

The respective transformation matrices are given as follows:

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

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

Now one has for the time derivative

$$\frac{\partial \boldsymbol{Q}}{\partial t} = \frac{\partial \boldsymbol{Q}}{\partial \tau}\frac{\partial \tau}{\partial t} = \frac{\partial \boldsymbol{Q}}{\partial \tau}\frac{1}{t^{n+1} - t^n} = \frac{1}{\Delta t}\boldsymbol{Q}_t, \tag{2.14}$$

and for the spatial derivative (Note: $\boldsymbol{x} = \begin{bmatrix} x & y & z \end{bmatrix}^T$ and $\boldsymbol{\xi} = \begin{bmatrix} \xi & \eta & \zeta \end{bmatrix}^T$)

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

furthermore

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

so that

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

where

$$
\left(\frac{\partial \boldsymbol{\xi}}{\partial \boldsymbol{x}} \right)_{ij} = \frac{\partial \boldsymbol{\xi}_i}{\partial \boldsymbol{x}_j}. \tag{2.18}
$$

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

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

where the modified flux is defined as

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

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

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

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

Lagrange basis function 1D:

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

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

Stiffness matrix:

$$\boldsymbol{K}_{ij} = \int_{T_E} \Phi_{i,\xi} \Phi_j d\boldsymbol{\xi}, \tag{2.24}$$

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

Mass matrix:

$$\boldsymbol{M}_{ij} = \int_{T_E} \Phi_i \Phi_j d\boldsymbol{\xi} \tag{2.25}$$

Chapter 3

Conclusion and Outlook

Chapter 4

Acknowledgment