



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

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Dr. Tobias Weinzierl
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Abstract

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Chapter 1

Introduction

Chapter 2

Theory

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 ν conserved quantities, and $\mathbf{F}(\mathbf{Q}) = (f, g, h)$ is a non-linear flux tensor that depends on the state \mathbf{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:

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

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 Ω , 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

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

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Transformation to space-time reference coordinate system (ξ, 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:

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

where the modified flux is defined as

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

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

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

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

Multiply the modified PDE (2.19) with space-time test function $\varphi_k = \varphi_k(\boldsymbol{\xi}, \tau)$ and integrate over the space-time reference element $T_E \times [0 : 1]$ to obtain the weak formulation:

$$\begin{aligned} \int_0^1 \int_{T_E} \varphi_k \frac{\partial Q}{\partial \tau} d\boldsymbol{\xi} d\tau + \int_0^1 \int_{T_E} \varphi_k \nabla_{\boldsymbol{\xi}} \cdot \mathbf{F}^*(Q) d\boldsymbol{\xi} = \\ \left\langle \varphi_k, \frac{\partial Q}{\partial \tau} \right\rangle + \langle \varphi_k, \nabla_{\boldsymbol{\xi}} \cdot \mathbf{F}^*(Q) \rangle = 0 \end{aligned} \quad (2.23)$$

Let the discrete solution in space and time \mathbf{q}_h and the discrete space-time representation of the flux tensor \mathbf{F}_h^* be defined as

$$\mathbf{q}_h = \mathbf{q}_h(\boldsymbol{\xi}, \tau) = \sum_l \varphi_l(\boldsymbol{\xi}, \tau) \hat{\mathbf{q}}_l := \varphi_l \hat{\mathbf{q}}_l \quad (2.24)$$

$$\mathbf{F}_h^* = \mathbf{F}_h^*(\boldsymbol{\xi}, \tau) = \sum_l \varphi_l(\boldsymbol{\xi}, \tau) \hat{\mathbf{F}}_l^* := \varphi_l \hat{\mathbf{F}}_l^*, \quad (2.25)$$

where the third expression in (2.24) and (2.25), respectively, make use of the Einstein summation convention, i.e. an index that appears exactly twice in an expression implies summation over this index.

Plugging (2.24) and (2.25) into the weak formulation (2.23) yields the discrete weak formulation

$$\left\langle \varphi_k, \frac{\partial \mathbf{q}_h}{\partial \tau} \right\rangle + \langle \varphi_k, \nabla_{\boldsymbol{\xi}} \cdot \mathbf{F}_h^*(\mathbf{q}_h) \rangle = 0. \quad (2.26)$$

We use space-time basis functions that are the tensor-product 1D Lagrange interpolation polynomials passing through the Gauss-Legendre quadrature points. The 1D basis functions are therefore defined as

$$L_i(\xi) = \prod_{j \neq i} \frac{\xi - \xi_j}{\xi_i - \xi_j}, \quad (2.27)$$

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

For two ($d = 2$) and three ($d = 3$) space dimensions the space-time basis functions on the space-time reference element $T_E \times [0; 1] = [0; 1]^{d+1}$ are then simply defined as

$$L_{ijk}(\boldsymbol{\xi}, \tau) = L_i(\xi) \cdot L_j(\eta) \cdot L_k(\tau) \quad (2.28)$$

$$L_{ijkl}(\boldsymbol{\xi}, \tau) = L_i(\xi) \cdot L_j(\eta) \cdot L_k(\zeta) \cdot L_l(\tau). \quad (2.29)$$

The d -dimensional tensor-product space-time basis is nodal, since the 1D basis functions are nodal, i.e. $L_i(\xi_j) = \delta_{ij}$, where δ_{ij} is the Kronecker delta defined as

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j. \end{cases} \quad (2.30)$$

As a result of using a nodal basis one has

$$\hat{q}_l = \hat{q}_h(\xi_l, \tau) = Q(\xi_l, \tau) \quad (2.31)$$

$$\hat{F}_l^* = F_h^*(\hat{q}_l) = F_h^*(q_h(\xi_l, \tau)) = F^*(Q(\xi_l)). \quad (2.32)$$

As a result of this choice of basis functions all resulting matrices are of sparse block structure and all computations can be done efficiently in a dimension-by-dimension fashion.

Integration by parts of the first term of the discrete weak formulation (2.23) yields

$$\begin{aligned} \left\langle \varphi_k, \frac{\partial q_h}{\partial \tau} \right\rangle &= \int_0^1 \int_{T_E} \varphi_k \frac{\partial q_h}{\partial \tau} d\xi d\tau = \\ &= \int_{T_E} \varphi_k q_h d\xi \Big|_{\tau=1} - \int_{T_E} \varphi_k q_h d\xi \Big|_{\tau=0} - \int_0^1 \int_{T_E} \frac{\partial \varphi_k}{\partial \tau} q_h d\xi d\tau = \\ &= [\varphi_k, q_h]_{\tau=0}^1 - \left\langle \frac{\partial \varphi_k}{\partial \tau}, q_h \right\rangle. \end{aligned} \quad (2.33)$$

Plugging (2.33) back into discrete weak formulation (2.23) yields

$$[\varphi_k, q_h]_{\tau=0}^1 - \left\langle \frac{\partial \varphi_k}{\partial \tau}, q_h \right\rangle + \langle \varphi_k, \nabla_{\xi} \cdot F_h^* \rangle = 0. \quad (2.34)$$

Taking into account the high order polynomial reconstruction $\mathbf{u}_h^n = \varphi_l \hat{\mathbf{u}}_l^n$ (???) in time step n as initial condition (in a weak sense) yields

$$[\varphi_k, q_h]_{\tau=1} - [\varphi_k, \mathbf{u}_h^n]_{\tau=0} - \left\langle \frac{\partial \varphi_k}{\partial \tau}, q_h \right\rangle + \langle \varphi_k, \nabla_{\xi} \cdot F_h^* \rangle = 0. \quad (2.35)$$

Substituting the ansatz (2.24) for the discrete solution $q_h(\xi, \tau)$ into (2.35) yields an implicit equation for the coefficients of the discrete solution \hat{q}_l :

$$[\varphi_k, \varphi_l]_{\tau=1} \hat{q}_l - [\varphi_k, \varphi_l]_{\tau=0} \hat{\mathbf{u}}_l^n - \left\langle \frac{\partial \varphi_k}{\partial \tau}, \varphi_l \right\rangle \hat{q}_l + \langle \varphi_k, \nabla_{\xi} \varphi_l \rangle \cdot F^*(\hat{q}_l) = 0, \quad (2.36)$$

where we used that (in Einstein notation)

$$\begin{aligned} (\nabla_{\xi} \cdot F_h^*)_i &= (\nabla_{\xi} \cdot (\varphi_l(\xi, \tau) F^*(\hat{q}_l)))_i = \frac{\partial (\varphi_l(\xi, \tau) F^*(\hat{q}_l))_{ij}}{\partial \xi_j} = \\ &= \varphi_l(\xi, \tau) \frac{\partial (F^*(\hat{q}_l))_{ij}}{\partial \xi_j} + (F^*(\hat{q}_l))_{ij} \frac{\partial \varphi_l(\xi, \tau)}{\partial \xi_j} = \\ &= (F^*(\hat{q}_l))_{ij} \frac{\partial \varphi_l(\xi, \tau)}{\partial \xi_j}, \end{aligned} \quad (2.37)$$

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i.e. in vector notation

$$\nabla_{\xi} \cdot \mathbf{F}_h^* = \nabla_{\xi} \cdot (\varphi_l(\xi, \tau) \mathbf{F}^*(\hat{\mathbf{q}}_l)) = \mathbf{F}^*(\hat{\mathbf{q}}_l) \cdot \nabla_{\xi} \varphi_l(\xi, \tau), \quad (2.38)$$

so that we can rewrite the last term of (2.35) as

$$\langle \varphi_k, \nabla_{\xi} \cdot \mathbf{F}_h^* \rangle = \langle \varphi_k, \nabla_{\xi} \varphi_l \rangle \cdot \mathbf{F}^*(\hat{\mathbf{q}}_l) \quad (2.39)$$

to finally obtain (2.36).

To finally obtain the coefficients $\hat{\mathbf{q}}_l$ of the discrete solution in space and time $\mathbf{q}_h = \varphi_l \hat{\mathbf{q}}_l$ we can use the following fixed-point iteration:

$$\left([\varphi_k, \varphi_l]_{\tau=1} - \left\langle \frac{\partial \varphi_k}{\partial \tau}, \varphi_l \right\rangle \right) \hat{\mathbf{q}}_l^{r+1} = [\varphi_k, \varphi_l]_{\tau=0} \hat{\mathbf{u}}_l^n - \langle \varphi_k, \nabla_{\xi} \varphi_l \rangle \cdot \mathbf{F}^*(\hat{\mathbf{q}}_l^r), \quad (2.40)$$

where $r = 0, 1, \dots$ is the iteration index. The solution $\hat{\mathbf{u}}^n$ of the previous time step can be used as a trivial initial guess, i.e.

$$\hat{\mathbf{q}}^0 = \hat{\mathbf{u}}^n, \quad (2.41)$$

the norm of the residual can be used as a termination criterion, e.g. stop the iteration if

$$R < \varepsilon, \quad (2.42)$$

where the residual R is defined as

$$R = \sqrt{(\hat{\mathbf{q}}^{r+1} - \hat{\mathbf{q}}^r)^T (\hat{\mathbf{q}}^{r+1} - \hat{\mathbf{q}}^r)} := \|\hat{\mathbf{q}}^{r+1} - \hat{\mathbf{q}}^r\|_2, \quad (2.43)$$

and $\varepsilon > 0$ is a constant chosen such that it reflects the desired accuracy of the complete computation.

TODO: Find matrices and understand when to integrate in time (-! Understand Picard iteration)

Stiffness matrix:

$$\mathbf{K}_{ij} = \int_{T_E} \Phi_{i,\xi} \Phi_j d\xi, \quad (2.44)$$

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

Mass matrix:

$$\mathbf{M}_{ij} = \int_{T_E} \Phi_i \Phi_j d\xi \quad (2.45)$$

To obtain a fully discrete one-step ADER-DG scheme proceed as follows:

-
- Multiply the original PDE (2.1) by a test function $\Phi_k \in \mathcal{U}_h \subset \mathcal{L}_\Omega^2 = \{u : \Omega \subset \mathbb{R}^{d+1} \rightarrow \mathbb{R} \mid \int_\Omega |u(x)|^2 dx < \infty\}$ which is identical with the spatial basis functions:

$$\Phi_k \frac{\partial Q}{\partial t} + \Phi_k (\nabla \cdot F(Q)) = 0. \quad (2.46)$$

- Integrate over space-time control volume $T_i \times [t^n, t^{n+1}]$:

$$\int_{t^n}^{t^{n+1}} \int_{T_i} \Phi_k \frac{\partial Q}{\partial t} dx dt + \int_{t^n}^{t^{n+1}} \int_{T_i} \Phi_k (\nabla \cdot F(Q)) dx dt = 0. \quad (2.47)$$

- Insert the discrete solution $\mathbf{u}_h = \hat{\mathbf{u}}_l \Phi_l$:

$$\int_{t^n}^{t^{n+1}} \int_{T_i} \Phi_k \frac{\partial \mathbf{u}_h}{\partial t} dx dt + \int_{t^n}^{t^{n+1}} \int_{T_i} \Phi_k (\nabla \cdot F(\mathbf{u}_h)) dx dt = 0. \quad (2.48)$$

- Integrate by parts the volume integral in the second term of (2.48):

$$\int_{T_i} \Phi_k (\nabla \cdot F(\mathbf{u}_h)) dx = \int_{T_i} \nabla \cdot (\Phi_k F(\mathbf{u}_h)) dx - \int_{T_i} F(\mathbf{u}_h) (\nabla \Phi_k) dx. \quad (2.49)$$

- Use the generalized divergence theorem for tensor fields [?, p. 954], i.e.

$$\int_\Omega \nabla \cdot \mathbf{U} dx = \int_\Omega \frac{\partial U_j}{\partial x_j} dx = \int_{\partial\Omega} \mathbf{U}_j \mathbf{n}_j dS \quad (2.50)$$

where \mathbf{U} is a tensor field with support support in Ω and \mathbf{n} is the outward pointing unit normal vector. Now let $\Omega = T_i$ and $\mathbf{U} = \Phi_k F(\mathbf{u}_h)$ so that for the first term on the right-hand side of (2.49) we have

$$\int_{T_i} \nabla \cdot (\Phi_k F(\mathbf{u}_h)) dx = \int_{\partial T_i} \Phi_k F(\mathbf{u}_h)_j \mathbf{n}_j dS. \quad (2.51)$$

- Insert (2.51) into (2.48) to obtain

$$\int_{t^n}^{t^{n+1}} \int_{T_i} \Phi_k \frac{\partial \mathbf{u}_h}{\partial t} dx dt + \int_{t^n}^{t^{n+1}} \int_{\partial T_i} \Phi_k F(\mathbf{u}_h)_j \mathbf{n}_j dS dt - \int_{t^n}^{t^{n+1}} \int_{T_i} F(\mathbf{u}_h) (\nabla \Phi_k) dx dt. \quad (2.52)$$

- As usual in the DG finite element framework replace the boundary flux term by a numerical flux function (Riemann solver) in normal direction, $\mathcal{G}(q_h^-, q_h^+)$, which is a function of the left and right boundary-extrapolated data, q_h^- and q_h^+ , respectively. Furthermore insert the

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local space-time predictor q_h and use the definition of the discrete solution $u_h = \Phi_l \hat{u}_l$ to obtain following arbitrary high order accurate one-step Discontinuous Galerkin (ADER-DG) scheme:

$$\begin{aligned} \left(\int_{T_i} \Phi_k \Phi_l dx \right) (\hat{u}_l^{n+1} - \hat{u}_l^n) + \int_{t^n}^{t^{n+1}} \int_{\partial T_i} \Phi_k \mathcal{G}(q_h^-, q_h^+)_j \cdot n_j dS dt - \\ \int_{t^n}^{t^{n+1}} \int_{T_i} F(q_h) (\nabla \Phi_k) dx dt = 0. \end{aligned} \quad (2.53)$$

TODO: Transformation $\int_{T_i} \Phi_k \Phi_l dx \rightarrow \int_{T_E} \Phi_k \Phi_l d\xi$ and other transformations

TODO: Limiting

TODO: Fallback method

Chapter 3

Conclusion and Outlook

Chapter 4

Acknowledgment
