Towards an exascale code for GRMHD on dynamical spacetimes

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Abstract. We present the first results on the construction of an exascale hyperbolic PDE engine (ExaHyPE), a code for the next generation of supercomputers with the objective to evolve dynamical spacetimes of black holes, neutron stars and binaries. We solve a novel first order formulation of Einstein field equations in the conformal and constraint damping Z4 formulation (CCZ4) coupled to ideal general relativistic magnetohydrodynamics (GRMHD), using divergence-cleaning. We adopt a novel communication-avoiding one-step ADER-DG scheme with an a-posteriori subcell finite volume limiter on adaptive spacetrees. Despite being only at its first stages, the code passes a number of tests in special and general relativity.

1. Introduction
Gravitational waves ejected by the merger of compact objects have been recently detected for both black hole-black hole mergers [1] as well as neutron star-neutron star mergers [2]. Both phenomena take place in the strong field regime of general relativity, described by Einstein field equations and so far only accessible by numerical relativity. The general relativistic fluid description of matter allows to predict precisely the dynamics of single and binary neutron stars. Furthermore, electromagnetism plays an important role for the realistic description of the fate of the binary system. General relativistic (magneto)hydrodynamics—in short GR(M)HD—is a successful theory to describe these phenomena, also underlying the gravitational wave banks used for the recently detected NS-NS merger.

The coupled numerical evolution of Einsteins and the GRMHD equations is a comparatively young field of research, as the first successful evolution of a BH-BH system dates back only one decade [3]. Since then, many GRHD and GRMHD codes for solving coalescing neutron stars have been developed (for instance [4–11], see also [12,13] for a review).

In the time of gravitational wave multi-messenger astronomy, the quantitative and qualitative need for accurate numerical simulations is essential. In the same time, computational science is entering the era of exascale computing, i.e. the first supercomputer to archive $10^{18}$ arithmetic operations per second is estimated to be built in the next three years. It is excepted that in order to reasonably exploit these resources, the next generation of numerical codes must satisfy tight constraints in locality, communication, storage, cache and energy efficiency [14].
In this work, we present ingredients for such a code which solves generic nonlinear hyperbolic first order balance laws,

$$\partial_t Q_k + \partial_i F^i_k(Q) + B^{ij}_k(Q)\partial_i Q_j = S_k(Q), \quad (1)$$

with a state vector $\vec{Q}$, conserved fluxes $\vec{F}^i$, a nonconservative part described by the matrix $\vec{B}^{ij}$ and algebraic source terms $\vec{S}$. We present particular PDEs, defined by $\{\vec{Q}, \vec{F}^i, \vec{B}^{ij}, \vec{S}\}$, as well as first results with actual implementations. The paper is structured as follows: In Section 2 we present the PDE system, in Section 3 we present the numerical scheme to solve this system, in Section 4 we present the grid representation and communication, in Section 5 we present first benchmarks and results while in Section 6 we give a summary and outlook of the next steps.

We work in geometric units (speed of light $c = 1$ and gravitational constant $G = 1$). Greek indices run from 0 to 3, Latin indices run from 1 to 3 and Einstein sum convention is applied over repeated indices. The signature of the metric tensor is assumed to be $(-, +, +, +)$.

2. The Einstein-Maxwell-Euler system

Three theories which describe a wide range of astrophysical phenomenae are

- Einstein equations
  $$R_{\mu\nu} + R_{\mu} = 8\pi G \, T_{\mu\nu}, \quad (2)$$
- Maxwell equations
  $$\nabla^\mu F_{\mu\nu} = 0 \quad \text{and} \quad \nabla^\mu F_{\mu\nu} = 0, \quad (3)$$
- Euler equations
  $$\nabla^\mu T_{\mu\nu} = 0 \quad \text{and} \quad \nabla_{\mu} (\rho u^\mu) = 0. \quad (4)$$

with Ricci scalar $R$, metric $g_{\mu\nu}$, energy momentum tensor $T_{\mu\nu}$, Faraday tensor $F_{\mu\nu}$, dual Faraday tensor $^*F_{\mu\nu}$, rest mass density $\rho$ and fluid velocity $u^\mu$. In the following, 3+1 initial value formulations in the language of (1) are presented.

2.1. A first order formulation of Einstein equations: FO-CCZ4

The formulation of Einstein equations used in this work builds upon successors of the original ADM Cauchy initial value formulation of Einstein equations [15] which introduces the 16 dynamical fields lapse $\alpha$, shift $\beta^i$, 3-metric $\gamma_{ij}$ and 3-extrinsic curvature $K_{ij}$. The ADM equations are not hyperbolic [16–18]. Two successors of the ADM equations are the BSSNOK formulation [19, 20] and the class of Z4 formulations [21, 22]. Both approaches were unified in the conformal and constraint-damping CCZ4 formulation [23, 24] which was recently rewritten in a first order formulation in space and time [25] which we subsequently refer to as FO-CCZ4. The full derivation and discussion of these equations including an eigenstructure analysis can be found in [25] where also strong hyperbolicity for the system in certain gauges is proven.

In order to briefly outline the equations, we introduce the conformal factor $\phi = (\det \gamma_{ij})^{-1/6}$ and subsequently $\gamma_{ij} = \phi^2 \gamma_{ij}$. We also define a conformal and trace-free extrinsic curvature tensor $\tilde{\gamma}_{ij} = \phi^2 (K_{ij} - \frac{1}{3} \gamma_{ij})$ where its trace $K = K_{ij} \gamma^{ij}$ has been seperated. Furthermore, we define the Christoffel variable contraction $\Gamma^i = \tilde{\gamma}^{ij} \tilde{\gamma}_{jk}$ as well as $\tilde{\Gamma}^i = \tilde{\Gamma}^i + 2 \tilde{\gamma}^{ij} Z_j$. Recall that $Z_{\mu} = (\Theta, Z_i)$ is the vector field which measures the distance to an analytical solution of Einsteins equations with constraint $Z_\mu = 0$. For the first-order formulation, we introduce the auxiliary vectors $A_i = \partial_i \ln \alpha$ and $P_i = \partial_i \ln \phi$ as well as tensors $B^i_i = \partial_k \beta^i$ and $D_{kij} = \frac{1}{2} \partial_k \tilde{\gamma}_{ij}$. Based on these quantities, the FO-CCZ4 system is given in Table 1 where system parameters $(\tilde{\gamma}, s, f, e, \kappa_{1,2,3}, c, \eta, \mu)$ and slicing condition $g(\alpha)$ are highlighted in red whereas matter contributions (cf. Section 2.2) are highlighted in blue. The state vector $\vec{Q}$ collects 59 evolved variables. For details on the imposed constraint equations, applied Bona-Massó gauge conditions and meaning of the parameters we refer again to [25].
\[ Q_i \]

| Table 1. FOCCZ4 system \( \partial_t Q + B(Q) \nabla Q = S(Q) \) |

| \( Q_i \) | NCPQ\(_i\): Nonconservative product \( B \nabla Q \) | \( S_Q\): Algebraic source \( S \) |
|---|---|---|
| \( \ln \alpha \) | \( 0 \) | \( \beta^k A_k - \alpha g(\alpha)(K - K_0 - 2\Theta c) \) |
| \( \beta^p \) | \( 0 \) | \( s^p B^p_k + s f \ell \) |
| \( \tau_{ij} \) | \( 0 \) | \( \beta^p 2 \delta_{ij} + \bar{\gamma}_k B^k_j + \bar{\gamma}_k B^k_i - 2 \bar{\gamma}_k \bar{\gamma}_i \bar{B}^{k} - 2a \bar{\gamma}_j \bar{A} \bar{A}_j - 2a \bar{\gamma}_j \bar{A} \bar{A}_j - \bar{\gamma}_j \bar{A} \bar{A}_j \) |
| \( \ln \phi \) | \( 0 \) | \( \beta^p P_k + \frac{1}{3} (aK - B^k_k) \) |

| Table 2. GRMHD system components |

| \( Q_i \) | Conserved Flux \( F^i \) | Nonconservative product \( B \nabla Q \) |
|---|---|---|
| \( D \) | \( w^D \) | \( 0 \) |
| \( S_j \) | \( \alpha W^j - \beta^p S_j \) | \( E \partial_t \alpha - \frac{\alpha}{2} g^{lm} \partial_j \gamma_{lm} - S_k \partial_j \beta^k \) |
| \( \tau \) | \( \alpha(S^s - w^D) - \beta^p \tau \) | \( S \partial^s \alpha - \alpha S \partial^s K_{ij} \) |
| \( B^j \) | \( w^B \beta^j - \partial_j \beta^k B^k + B^k j \beta^j \) | \( \phi \partial^j \beta^j + \frac{1}{2} \psi (\chi^j \beta^j \gamma_{ij} - B^j \partial_j \alpha) \) |
| \( \phi \) | \( \phi - \alpha B^k \) | \( \phi \partial \beta^j + \frac{1}{2} \psi (\chi^j \beta^j \gamma_{ij} - B^j \partial_j \alpha) \) |

2.2. The GRMHD system

The GRMHD system describes general relativistic hydrodynamics coupled to the magnetohydrodynamic approximation of Maxwell theory where magnetic field lines are advected with the fluid and the electric field is given by \( \vec{E} = -\vec{v} \times \vec{B} \). This, the Maxwell equations reduce to an evolution equation for the magnetic field as well as the constraint equation \( \nabla \cdot \vec{B} = 0 \).

Violations are treated with a cleaning approach, i.e. we evolve an additional scalar field \( \phi \) to transport constraint violations (no damping is applied). The PDE system is given in Table 2, where \( D = W \) is the conserved density which is related to the rest mass density \( \rho \) by the Lorentz factor \( W = (1 - v^2)^{-1/2} \) with fluid velocity \( v \). The conserved momentum is given by \( S_j = \rho W^2 v_j \). We also evolve the rescaled energy density \( \tau = E - D = \rho W^2 - p - W \) where \( E \) is the energy density measured by the Eulerian observer and \( p \) is the fluid pressure. \( B^i \) represents the magnetic field and \( w^k = \alpha v^k - \beta^k \) the advection velocity relative to the coordinates, also referred to as transport velocity. The GRMHD 3-energy-momentum tensor is given by \( S^{ij} = S^i v^j + (p - T_k^k / 2) - T^{ij} \) with \( T^{ij} = B^k B^j / W^2 + (B^i v^j)(B^k v_k) \) the Maxwell 3-energy momentum tensor. The primitive recovery follows [26–28]. Note that all fields are rescaled to a tensor density by \( \sqrt{g} \equiv \sqrt{\text{det} g_{ij}} \) and the actual PDE therefore reads

\[
\partial_t \sqrt{g} Q_i + \nabla_j \sqrt{g} F^j(Q) + \sqrt{g} B \nabla Q = 0 .
\] (5)

For a comprehensive discussion of this system in context of our ADER-DG approach (Section 3), we refer to our publication [29].
3. Communication-avoiding ADER-DG scheme with a subcell limiter

We adopt a path-conservative arbitrary high order derivative discontinous Galerkin (ADER-DG) scheme with a finite volume (FV) limiting approach, adaptive mesh refinement (AMR) and local timestepping. This scheme was already applied on several nonrelativistic problems [11, 30–32] and recently formulated for GRMHD [29].

The computational (spatial) domain $\Omega$ is covered by Cartesian nonoverlapping cells $\Omega_i$ (also referred to as patches or elements). The analytic DG solution $u_h(x, t^n) = \sum_l \hat{u}^n_{kl} \Phi_l(x)$ is written in an orthogonal basis $\Phi_l(x)$ in each cell. We choose the Euler-Legendre polynomial basis at order $N$ and thus store $N+1$ degrees of freedom (DOF) on a non-uniform nodal subgrid. The PDE system (1) is multiplied by these spatial test functions and written in weak integral form as

$$0 = \int_{t^n}^{t^{n+1}} \int_{\Omega_i} dx \left( \frac{\partial Q}{\partial t} + \frac{\partial F^i(Q)}{\partial x^i} + B^{ij} \frac{\partial Q_j}{\partial x^i} - S(Q) \right) \Phi_k. \quad (6)$$

3.1. Space-time predictor

In order to achieve element-locality, the scheme (6) is separated in an element-local space-time predictor and a corrector step where boundary face values are communicated,

$$0 = (\hat{u}^{n+1}_{kl} - \hat{u}^n_{kl}) M_{kl} + \int_{t^n}^{t^{n+1}} \int_{\partial \Omega_i} dS \Phi_k \mathcal{J}(q_h^{-}, q_h^{+}) + \int_{\Omega_i \setminus \partial \Omega_i} dx \Phi_k [B(q_h) \nabla q_h - S]. \quad (7)$$

Here, the $q_h$ is the element-local predictor solution and $M_{kl} = \int_{\Omega_i} dx \Phi_k \Phi_l$ the diagonal element mass matrix. The surface integral collects the conservative and nonconservative jump terms $\mathcal{J}$ between cells and is subject of an approximate Riemann solver, we apply a path-conservative HLLEM method [33] which takes the nonconservative terms into account.

The predictor solution $q_h(x, t)$ is approximated in time from a known solution without considering the interaction with the neighbouring cells. We thus solve a local Cauchy problem inside the cell,

$$\int_{t^n}^{t^{n+1}} \int_{\Omega_i} dx \Theta_k(x, t) \left( S(q_h) - B^{ij} \nabla q_h - \nabla F(q_h) \right) = \int_{t^n}^{t^{n+1}} \int_{\Omega_i} dx \Theta_k(x, t) \frac{\partial q_h}{\partial t}, \quad (8)$$

$$= \int_{\Omega_i} dx \Theta_k(x, t^{n+1}) (q_h(x, t^{n+1}) - u_h(x, t^n)) - \int_{t^n}^{t^{n+1}} \int_{\Omega_i} dx \frac{\partial \Theta_k}{\partial t} q_h(x, t), \quad (9)$$

which was rewritten by partial integration in order to achieve a fixed-point problem which can easily be solved with fast converging algorithms [34, 35].

3.2. Subcell limiter

In case of discontinuities in the solution, the ADER-DG scheme can produce spurious oscillations (Gibbs phenomena) or even unphysical solutions. We encounter these problems by switching to a robust finite volume scheme on a regular subgrid. This switch is either done a priori on a purely geometrical criterion (e.g. static puncture position) or a posteriori, after computing a DG timestep. In the latter case, several criteria are applied to ensure the correctness of the solution: Mathematical admissibility criteria (the occurrence of floating point errors), physical
admissibility criteria (e.g. $D > 0$, $\vec{v}^2 < 1$, $\rho > 0$ in the GRMHD equations or $\alpha < \alpha_0$ in CCZ4) as well as an heuristic discrete maximum principle (DMP) which checks whether all cell solutions are below the maxima and above the minima of the adjacent cells.

By choosing a subgrid size of $M = 2N + 1$ cells per axis, where $N$ is the order of the DG polynomial, the number of subcells is maximized without breaking the CFL condition which would make the limited cells evolve with smaller timesteps than untroubled DG cells. We can not only preserve all $N + 1$ DOF per axis of a troubled DG cell, the limiter also acts as a natural mesh refinement on its own.

In principle, any FV scheme can be used. We implemented an ADER-TVD [29] and ADER-WENO scheme [25] but also, for communication avoidance, a 1st order Godunov scheme and a 2nd order MUSCL-Hancock scheme [36]. The limiter is extensively described in the references [25, 29, 36]. In short, it completely replaces the DG scheme in the troubled cell. In order to properly communicate the boundary values, a DOF prolongation of DG→FV is also necessary in the adjacent cells. After each timestep, the restriction FV→DG takes place to restore the DG polynomial.

4. Exascale architecture

It is assumed that many assumptions of contemporary high performance computing no longer hold at the exascale. For instance, due to the heterogeneity and complex, error-prone and fault-tolerant computer architectures, equal work distribution (i.e. naive Cartesian slicing which minimizes the allocation surface) is no longer assumed to lead to balanced computing time. Similarly, massive parallel scalability will become even more important, and thus the communication overhead has to be reduced at any price [14].

4.1. Separation of physics and machinery: Loose of control

Cactus and the Einstein Toolkit [37, 38] are examples of mature frameworks for PDE solvers. While they focus on abstracting the distributed memory parallelization (MPI), the advent of manycore processors requires hybrid codes (shared memory parallelization, e.g. OpenMP or TBB) and diffused the clear separation of physics and computational infrastructure [39, 40]. In contrast, the novel ExaHyPE code forces the users to step back from implementing random access schemes as it prescribes both the data layout, programming workflow as well as the major algorithmic steps [36, 41, 42]. Primarily, the physicist as a user declares the PDE system without describing its control flow.

4.2. Spacetime AMR by Peano

We use the Peano framework [43] which implements tree-structured Cartesian meshes with adaptive mesh refinement (AMR). The name indicates that the Peano space filling curve is employed for storage locality [44]. The code also supports Hybrid (MPI and TBB) parallelization with dynamic load balancing.

Peano implements the inversion of control paradigm where users give up control of the program workflow in order to profit from high-level task restructuring. Peano defines the program workflow in terms of two coupled finite state machines, one for the grid traversal and one for the major steps of the PDE solver. Peano is one of the building blocks of the exascale hyperbolic PDE engine ExaHyPE [41]. In ExaHyPE, the concrete numerical scheme (e.g. the particular Riemann solver used) is exchangeable and delegated to modular kernels which can be tailored to a specific PDE.

5. Benchmarks and Results

This section collects separated results from vacuum spacetime [25], GRMHD in fixed background Cowling approximation [29], and dedicated nonrelativistic tests with the limiter in the Peano
framework [36]. All figures are taken from the respective publications. The evolved fluids follow an ideal gas equation of state.

5.1. Nonrelativistic benchmarks
Figure 1 visualizes the Limiter functionality on an Eulerian explosion problem (spherical Sod shock tube [45, 46]). Figure 2 shows a similar but non-spherical Sod shock tube. Both figures highlight the transition steps between limited (troubled) cells and unlimited cells. Figure 3 shows the 2D SRMHD rotor problem [47] in a poor resolution, cf. [31, fig. 4] for a high resolution. Since the limiter acts only per-cell, a minimum resolution is necessary to properly work.

![Figure 1](image1.png)  
**Figure 1.** Radial explosion problem with clearly visible cell status.  

![Figure 2](image2.png)  
**Figure 2.** 2D Sod shock tube. The rarefaction wave and shock front are computed with ADER-DG, only the contact discontinuity is limited.  

![Figure 3](image3.png)  
**Figure 3.** MHD Rotor, poorly resolved: Coincidental limiting due to heuristics.

5.2. Cowling GRHD benchmarks
Figure 4 shows the Limiter active in a 2D thick torus [48] solution after $t = 1000M$. Figure 5 shows the grid around a TOV [49] neutron star surface. Both figures show the color encoded rest mass density profile. The limiter always activates at the sharp crossover from matter to vacuum (atmosphere).

![Figure 4](image4.png)  
**Figure 4.** 2D thick torus in polar coordinates. The red cells indicate limited cells.  

![Figure 5](image5.png)  
**Figure 5.** 3D cut of a stable neutron star. Green cells indicate limited cells on a 3-level AMR grid.
5.3. Vacuum spacetime benchmarks
Figure 6 shows the Hamiltonian and momentum constraint violations during the evolution of a static Schwarzschild black hole spacetime with the FO-CCZ4 system. Limiting is applied only in the vicinity of the puncture. Figure 7 shows a smooth gauge wave after 160 crossing times which is recovered with 100 cells at third order \( p = 3 \) already very good.

![Figure 6. Errors in the black hole spacetime evolution up to \( t = 1000M \).](image)

![Figure 7. Large amplitude gauge wave](image)

6. Summary
We have shown first results on a new code which is the unification of three different scientific branches: The development of a new formulation of Einstein Equations, the application of sophisticated high-order schemes and the implementation in a pioneering high performance grid framework.

The proposed novel first order CCZ4 formulation was proven to be strongly hyperbolic. Due to the special treatment of the nonconservative terms as Borel measures, the system can be evolved very accurately. The dynamical coupling of CCZ4 and GRMHD were sketched and are subject to ongoing investigations.

The ADER-DG scheme provides high order time integration and high order space discretization. The local space-time predictor is communication avoiding and allows to integrate with only one data transfer/grid traversal per time step [36]. The goal is to maximize the arithmetic intensity (“science per watt”). The subcell limiter preserves the degrees of freedom by resolving physical oscillations with adaptive mesh refinement. It is shock capturing as it allows to evolve shock fronts stably with any finite volume scheme.

The Peano framework provides a modern AMR framework where users give up control in order to obtain scalability and maintainability. Peano promises scaling to millions of cores. All together, the three ingredients (i) CCZ4+GRMHD (ii) the communication avoiding ADER-DG and (iii) Peano, were merged to a single code called ExaHyPE from which first results have been shown in this work and more are expected soon.

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