The ExaHyPE Hyperbolic PDE-Engine: Mesh generation avoiding schemes for the Earthquake simulation in Alpine Regional Areas.

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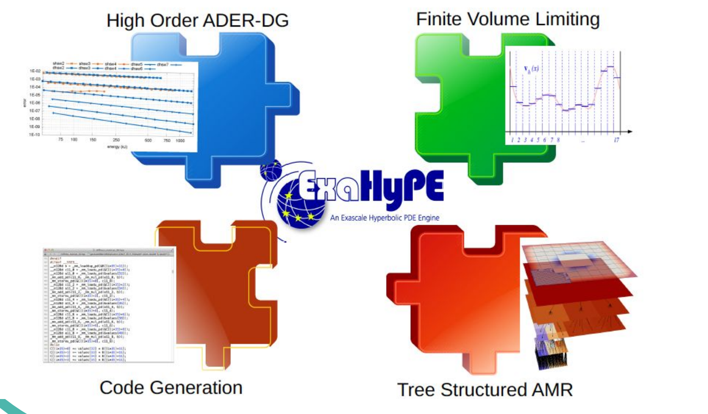
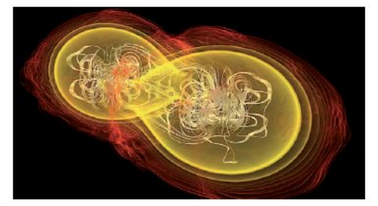
ADER-DG as Exascale Hyperbolic PDE Engine

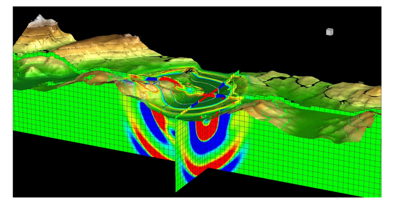
ExaHyPE (www.exahype.eu) is an open source software to solve hyperbolic PDE systems stemming from conservation laws (as arising in seismology, astrophysics, fluid dynamics, etc.). This hyperbolic PDE Engine (as in game "engine") is designed for exascale supercomputers of tomorrow (10^{18} FLOPs/sec).

Key assumption: We assume that exascale simulations will **require tailoring** of existing codes to specific grand challenge applications, but may **exploit** general-purpose algorithmic solutions, such as provided by our **engine**. Exascale size problems can only be tackled by fully **automatized representation of complexities** - without manual user interaction.

Key goals: i) Enable medium size interdisciplinary research team to realize extreme scale applications tackle grand challenge simulations quickly; ii) Efficiently solve hyperbolic PDEs on **Cartesian grids with high-order ADER-DG schemes and finite volume subcell limiters**

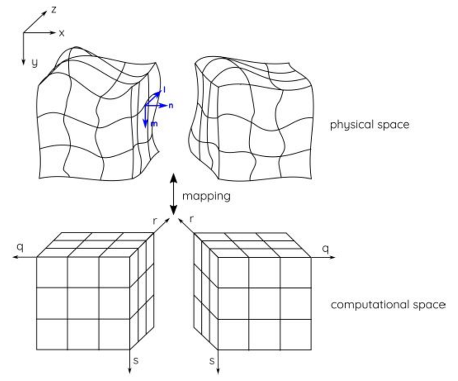


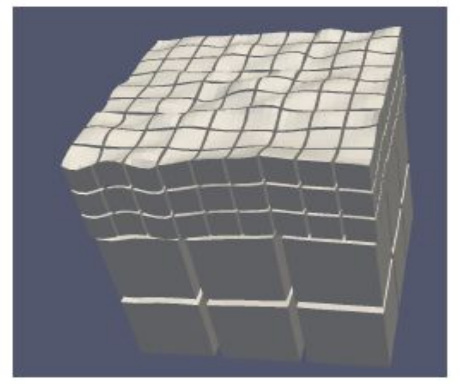


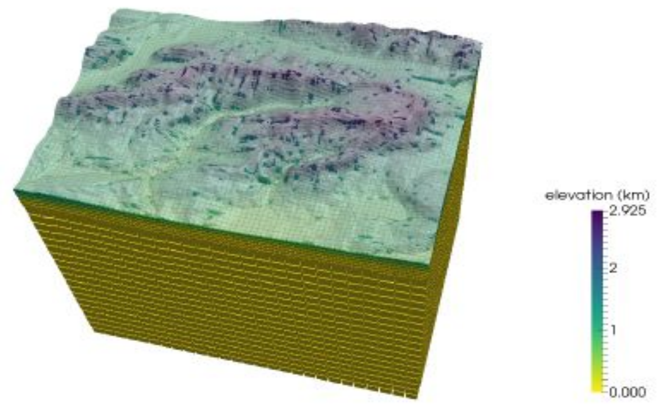


Currently two pioneering application fields:
Astrophysics (merging neutron stars);
Computational seismology (earthquake rupture dynamics)

Adaptive Curvilinear Mesh and Transformation







Implicit embedding of curvilinear meshes in adaptive Cartesian meshes. Elements are connected and boundary conditions are imposed using physics based numerical fluxes.

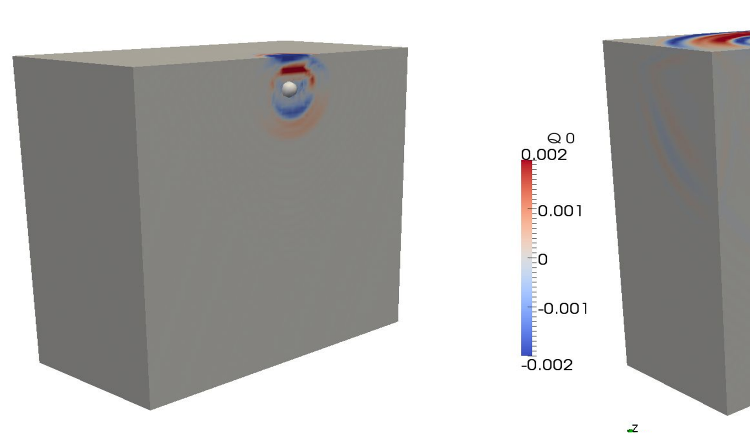
$$\int_{\tilde{\Omega}} \phi^T \widetilde{\mathbf{P}}^{-1} \frac{\partial}{\partial t} \mathbf{Q} dq dr ds = \int_{\tilde{\Omega}} \phi^T \left(\nabla \cdot \mathbf{F}(\mathbf{Q}) + \mathbf{B}(\nabla \mathbf{Q})\right) dq dr ds$$
$$- \sum_{\xi = q,r,s} \int_{\tilde{\Gamma}} \sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2} \left(\left[\phi^T \mathbf{FL}\right]_{\xi=0} + \left[\phi^T \mathbf{FR}\right]_{\xi=1} \right) J \frac{dq dr ds}{d\xi}.$$

We use structure preserving coordinate transformations to transform the PDE from the physical space to the computational space. **FL** and **FR** are physics based flux fluctuations designed to satisfy the physical phenomena (including nonlinear friction laws) occurring at element faces. Together the transformations and the numerical flux fluctuation satisfy the energy equation.

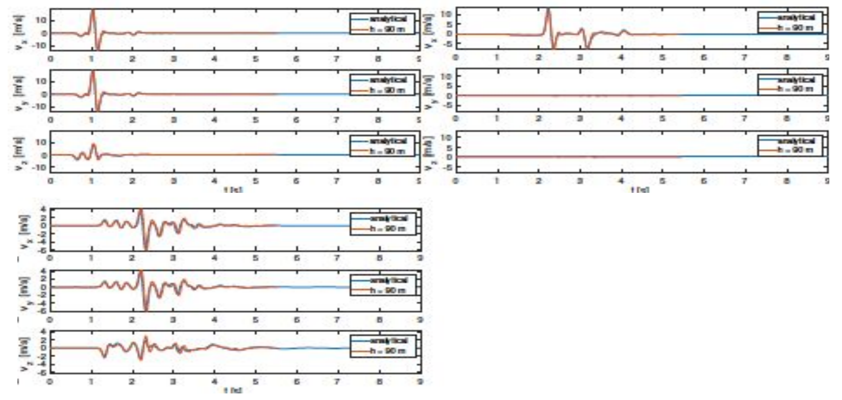
$$\frac{d}{dt}\left(E^-(t) + E^+(t)\right) = IT_s\left(\hat{v}^{\pm}, \hat{T}^{\pm}\right) + BT_s\left(\hat{v}^-, \hat{T}^-\right) + BT_s\left(\hat{v}^+, \hat{T}^+\right) + F_{luc}\left(G^-, Z^-\right) + F_{luc}\left(G^+, Z^+\right) \le 0.$$

Seismic Wave propagation

We accurately solve the layer over a homogeneous half space benchmark (LOH1)



Snapshots of the wavefields at 1 s and 5 s.

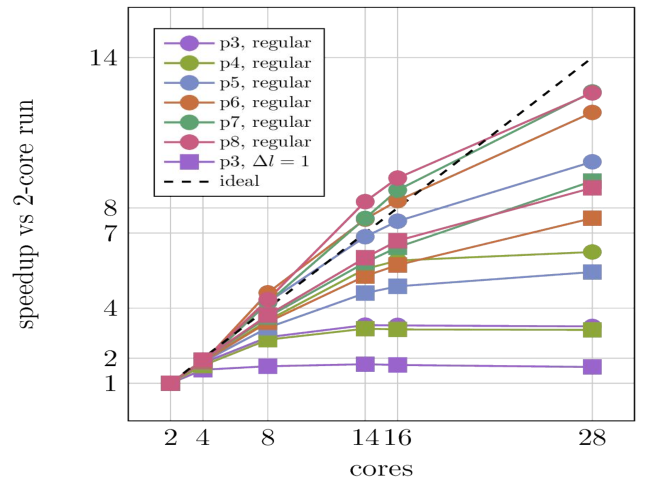


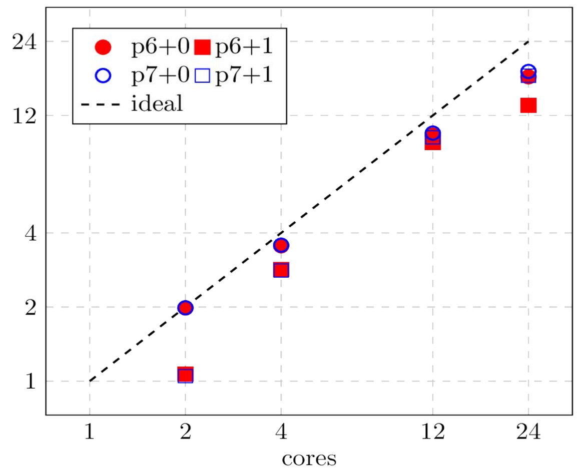
Comparisons of seismograms at three different stations

Core Level Optimization

- **ExaHyPE**'s key idea is to use tailored, extremely optimised code routines using SIMD vectorisation and architecture specific matrix operations.
- Using these optimisations ExaHyPE achieves **13% of peak performance** on Skylake architectures with an extremely **high level of vectorisation**.

Shared-memory scalability of the ADER DG implementation on SuperMUC phase 2 for the LOH1 benchmark. The grid consists of 27^3 cells and one level of dynamically refined cells in the layer above the halfspace.





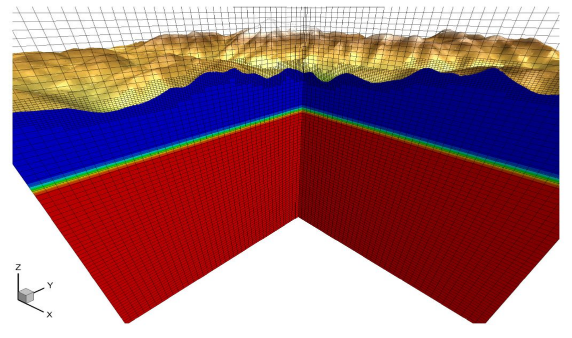
Distributed-memory scalability of the ADER DG implementation on the Hamilton cluster for the LOH1 benchmark. The grid consists of 27^3 cells.

New Diffuse Interface Approach for Complex Geometries

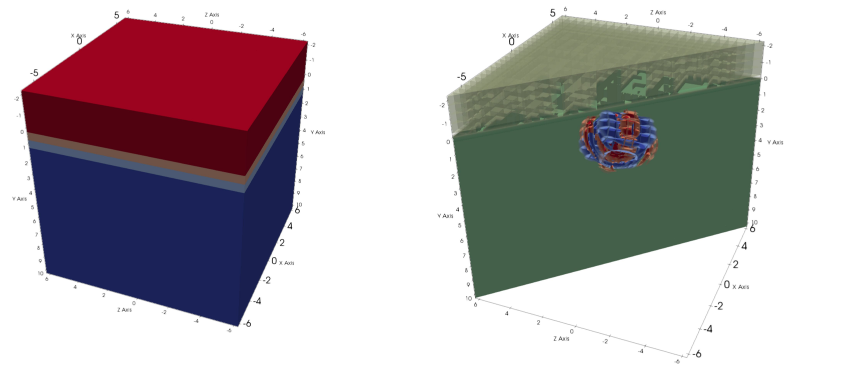
- Representation of general non grid-aligned geometries via the new diffuse interface method using ADER-DG schemes with subcell FV limiter on AMR grids is very simple. Inside the solid one sets α = 1, and α = 0 outside
- We exploit the fact that the DIM reduces to the basic Elastic Wave Equation for α = 1 and solve solid areas with the computationally cheaper Cauchy Kovalevskaya method.
- The jump from α = 1 to α = 0 is rapid, we thus solve two problems at once: We can apply multiple solvers with help of the engines Finite Volume limiter and resolve oscillations due the discontinuity with the more stable

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} - \mathbf{E}(\lambda,\mu) \cdot \frac{1}{\alpha} \nabla(\alpha \boldsymbol{v}) + \frac{1}{\alpha} \mathbf{E}(\lambda,\mu) \cdot \boldsymbol{v} \otimes \nabla \alpha = \boldsymbol{S}_{\sigma},$$
$$\frac{\partial \alpha \boldsymbol{v}}{\partial t} - \frac{\alpha}{\rho} \nabla \cdot \boldsymbol{\sigma} - \frac{1}{\rho} \sigma \nabla \alpha = \boldsymbol{S}_{v},$$
$$\frac{\partial \alpha}{\partial t} = 0.$$

Final governing PDE system written in non-conservative form

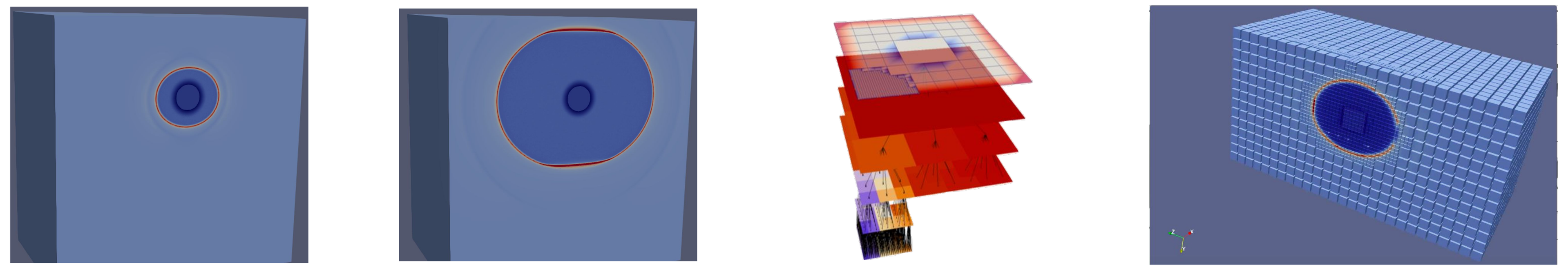


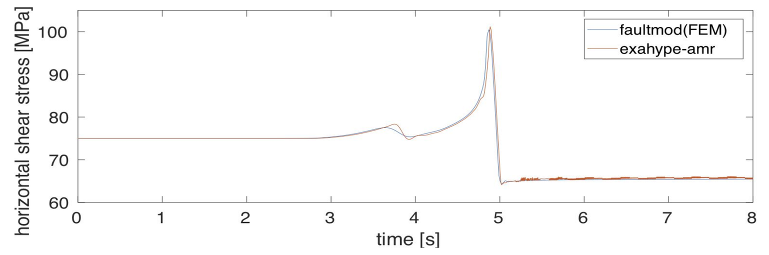
Fully automatic setup of the test problem based on real DTM data. All that is needed is to specify the volume fraction function.



Loh1 with the DIM at t = 0.4s (Right)
The Surface is limited by the subcell Finite Volume Limiter (Left)

Multi-physics: Non-linear Dynamic Rupture Coupling

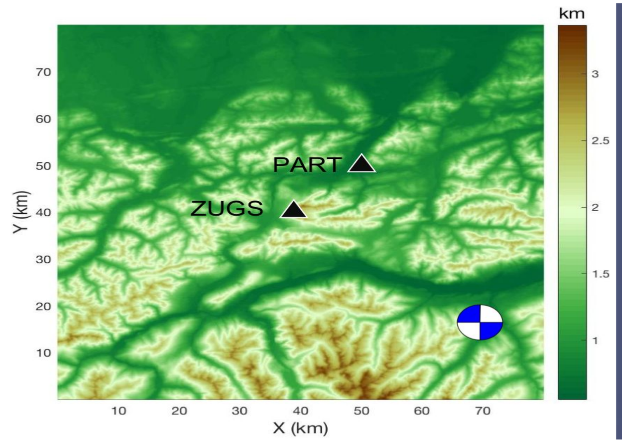


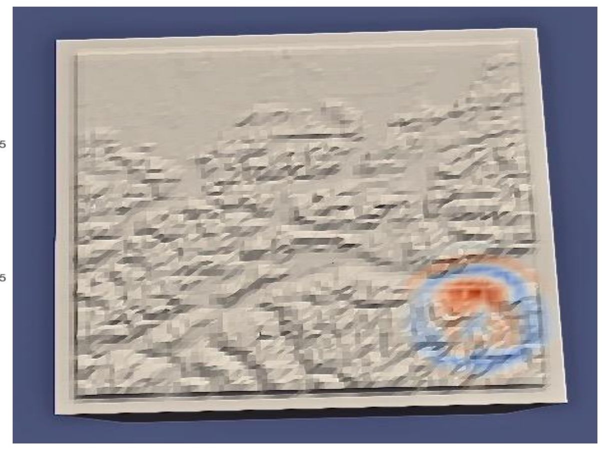


Top panel: Snapshots showing the evolution of the shear stress on the fault.
Left panel: A comparison with the finite element model.

- We verify ExaHyPE in a 3D SCEC dynamic rupture benchmark problem (TPV101) by solving the spontaneous dynamic rupture problem on a static AMR mesh. The fault is governed by the nonlinear rate-and-state friction law, and the state variable evolves according to the aging law.
- We explore 3D dynamic AMR to accurately capture the rupture tip and wave fronts

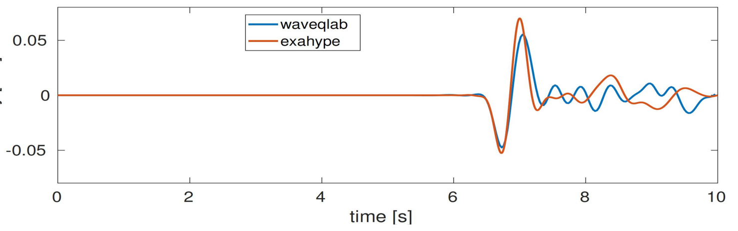
Zugspitze Scenario: Topography Shielding/Amplification





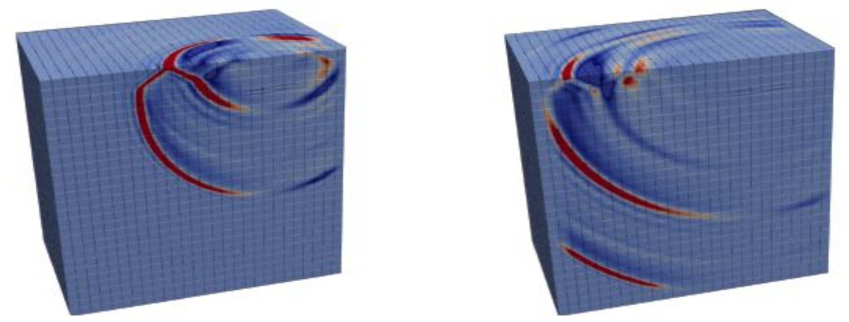
An ExaHyPE simulation with 27 elements and GLL nodes. The figure shows wave propagation at 2s.

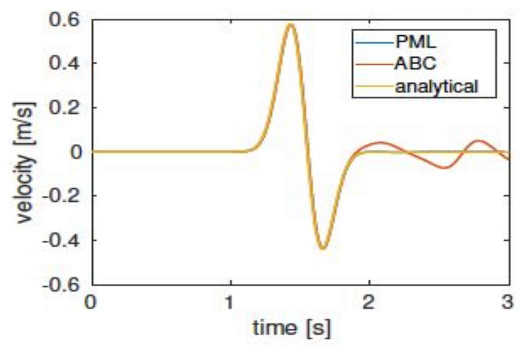
- Targeting regional scale seismic hazard scenarios (e.g. AlpArray): We design a scenario in a 80x80x80 km domain with high-resolution topography centered at Mount Zugspitze, Germany, to study the impact of surface topography on seismic



Waveform comparison at station ZUGS between preliminary WaveQLab3D simulations and ExaHyPE.

Perfectly Matched Layer (PML)





We verify the accuracy and stability of the PML absorbing boundary condition in elastic media with free-surface boundary conditions.

- **ExaHyPE combines:** a novel, physics-based numerical flux accurately representing surface waves, dynamic rupture boundary condition, curvilinear meshes via multi-block boundary conforming with AMR, provable stable PML boundary conditions, parallel handling of input data for material parameters and topography via a geoinformation server (ASAGI, Rettenberger et al. 2016)
- **Future work:** We will develop criteria and error estimates to exploit dynamic AMR features of the ExaHyPE Engine, compare time to solution of the curvilinear method against established and novel numerical schemes for the Elastic Wave Equation (e.g. Diffuse Interface Method (Tavelli et al., JCP 2018); we plan an **"ExaSeis"** release consolidating the computational seismology applications. We will further improve scalability.

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