CHEESE

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Center of Excellence for Exascale in Solid Earth

Seismic Simulations using the ExaHyPE Engine

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The ExaHyPE Project

- EU Horizon 2020 project in the FETHPC call
  "Towards Exascale High Performance Computing"
  (New mathematical and algorithmic approaches)
- ExaHyPE has received followup funding through *ChEESE*
  The main objective of ChEESE is to establish a new Center of Excellence (CoE) in the domain of Solid Earth (SE) targeting the preparation of 10 Community flagship European codes for the upcoming pre-Exascale (2020) and Exascale (2022) supercomputers.

People

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- **Instructors:** Leonhard Rannabauer,
  Philipp Samfass, Lukas Krenz, Mario Wille





Towards an Exascale Hyperbolic PDE Engine

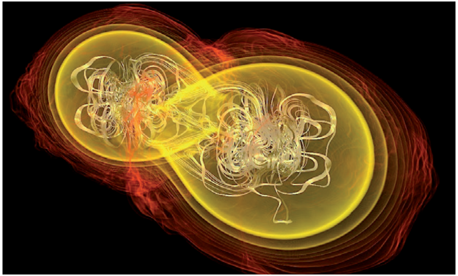
ExaHyPE Goal: a PDE "engine" (as in "game engine")

- enable medium-sized interdisciplinary research teams to realise extreme-scale simulations of grand challenges quickly
- efficiently solve hyperbolic PDE systems on Cartesian grids using higher-order ADER DG schemes with subcell limiting

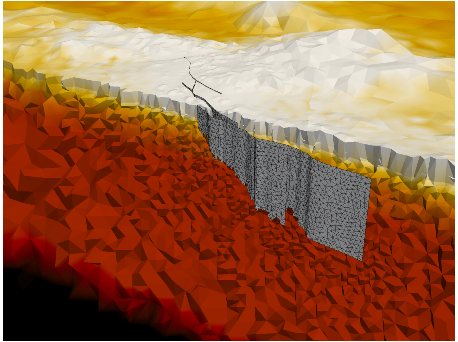
Towards an Exascale Hyperbolic PDE Engine

- primary focus on two application areas:

Astrophysics



Seismology



Hyperbolic PDE systems

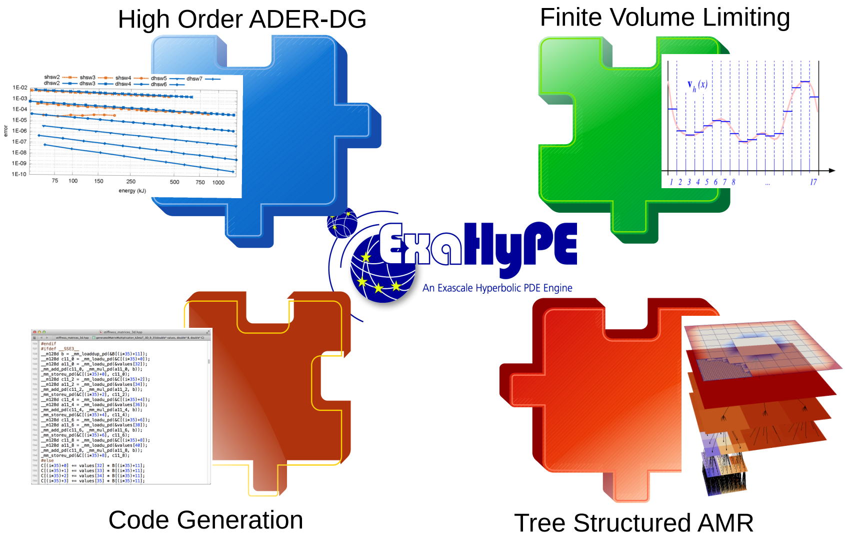
The ExaHyPE Engine solves systems of first-order hyperbolic PDEs in the following form:

$$P\frac{\partial Q}{\partial t} + \nabla \cdot F(Q) + \sum_{i=1}^{d} B_i(Q)\frac{\partial Q}{\partial x_i} = S(Q) + \sum \delta,$$

with

- material matrix P
- state vector Q
- conserved flux vector F
- non-conservative fluxes $\sum B_i(Q)\frac{\partial Q}{\partial x_i}$
- algebraic source terms S
- point sources $\sum \delta$

The ExaHyPE Engine



Engine Architecture and Application Interface

Application Layer – user provides:

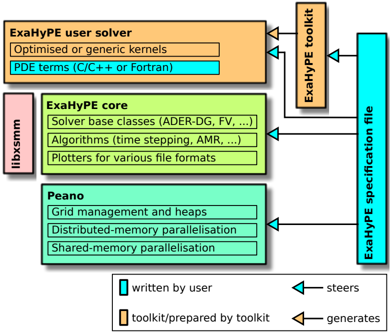
- C/Fortran code for fluxes: $F(Q)$, $G(Q)$, etc.
- C/Fortran code for eigenvalues: $\lambda_1 = u + \sqrt{gh}$, etc.

ExaHyPE toolkit generates:

- core routines, templates for application-specific functions
- kernels tailored to discretisation order, number of quantities, etc.

Peano framework:

- hybrid MPI+Intel TBB parallelism
- data structures for parallel AMR



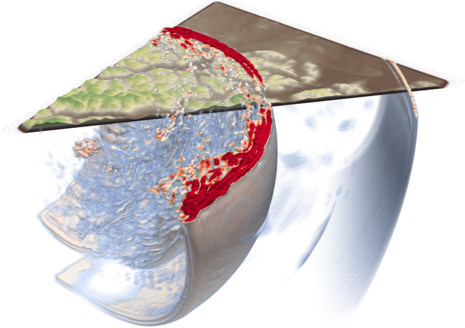
Available Equations

The Flexibility of the Engine allows the implementation of highly different PDE systems:

- Euler Equations
- **Tsunamis with the Shallow Water Equations**
- **Curvilinear Meshes for the Elastic Wave Equation**
- **Diffuse Interface Approach**
- **Perfectly Matching Layers for the Elastic Wave Equation (PML)**
- Clouds with the Compressible Navier-Stokes Equations
- General Relativistic Magneto-Hydrodynamics
- **Godunov-Peshkov-Romenski (GPR) Model**
- Gravitational waves with the Einstein's Equations in Vacuum

Curvilinear Meshes

K. Duru and L. Rannabauer



- Maps each element from Cartesian mesh onto a boundary fitting curvilinear mesh.
- Requires initial mesh generation which we automated based on a simple k-d-tree approach.
- Flux and source terms are transformed with the Jacobian.
- Eigenvalues and time-step size highly depend on the norm of the transformation.

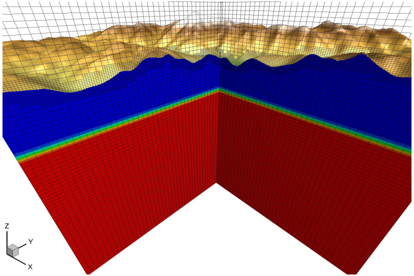
Diffuse Interface Approach

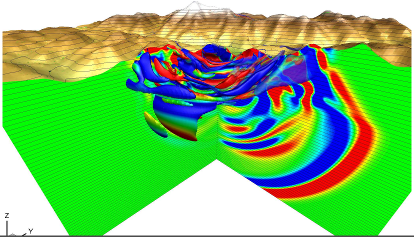
M. Tavelli and M. Dumbser

Idea: Introduce a parameter α, which identifies the location of solid medium

$$Q = \begin{pmatrix} \sigma & \alpha v & \lambda & \mu & \rho & \alpha \end{pmatrix}^T,$$
$$\partial_t \alpha = \partial_t \lambda = \partial_t \rho = \partial_t \mu = 0$$

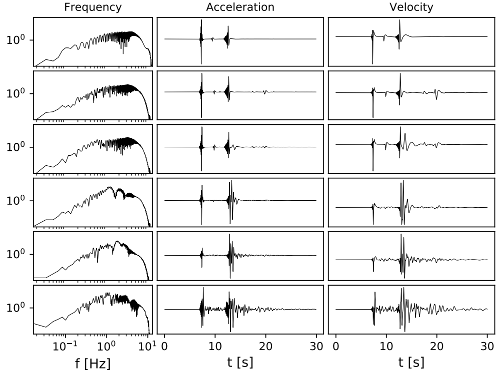
- At boundaries fluxes are *no longer linear*.
- This new approach *completely avoids* the problem of mesh generation
- The eigenvalues and time-step size are *independent* from the topography.
- Allows moving meshes

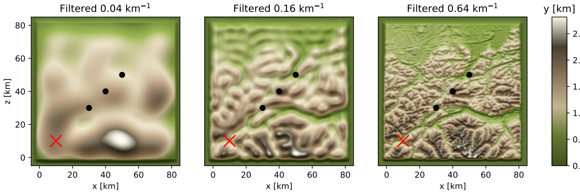




Scattering Effects in the Alpine Region

K. Duru and L. Rannabauer



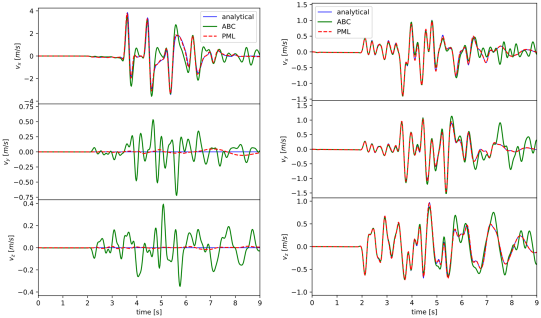


Goal: Track topographic effects on wave scattering.

- Filter topography for different cut-off frequencies
- Conclude on frequency content in Coda waves

Perfectly Matched Layers

K. Duru and L. Rannabauer

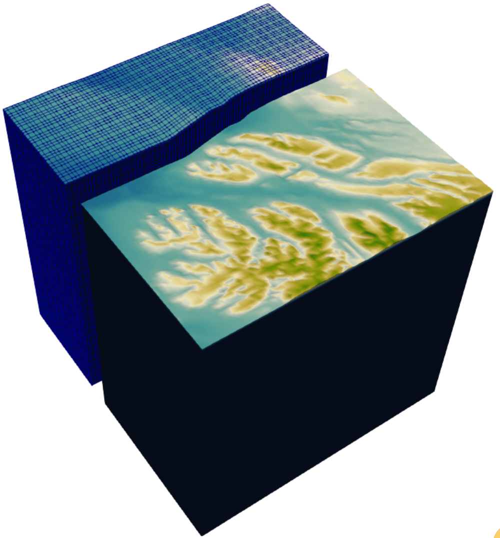


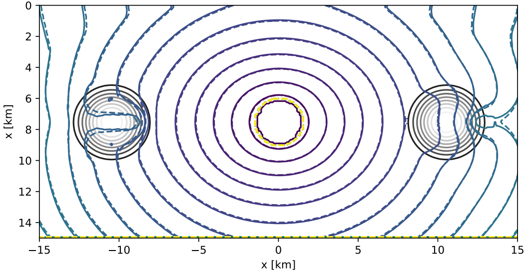
Goal: Remove reflections emanating from the not perfectly absorbing boundary of the computational domain.

- Based on complex coordinate stretching.
- Requires extension of the numerical DG fluxes, inter-element and boundary procedures.
- Allow us reduce the the computational domain and only simulate the area of interest.

Multipyhsics Dynamic Rupture

K. Duru et al.

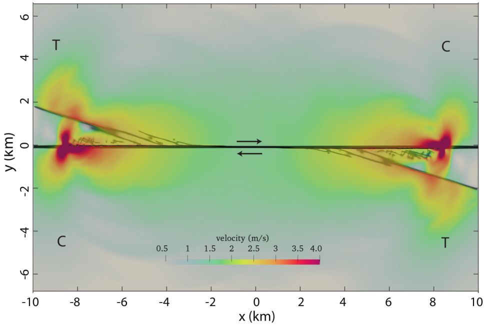




- Novel non-linear interface conditions and dynamic adaptive mesh refinement in 3D.
- Rupture is incorporated as boundary condition in a newly developed pyhsics based Riemann solver.

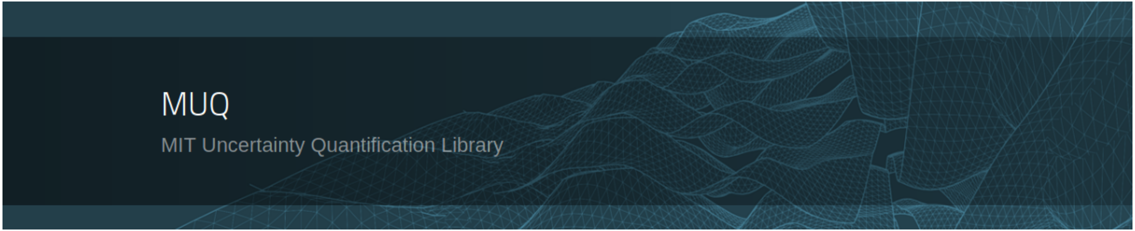
GPR: Godunov, Peshkov and Romenski model

AA. Gabriel, D. Li



Goal: Numerical modeling of continuous damage and freely evolving dynamic rupture.

- Based on the Godunov Peshkov Romenski, a unified framework for arbitrary rheological responses of material.
- Used for nonlinear elasto-plasticity, material damage and of viscous Newtonian flows with phase transition between solid and liquid phases.
- Fault geometry and secondary cracks are part of the PDE.
- A scalar function $\xi \in [0, 1]$ indicates the local level of material damage.



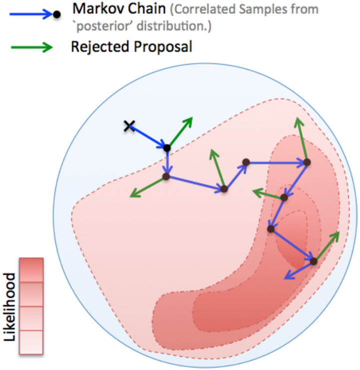
The MUQ library is a C++ toolbox for uncertainty quantification

Features:

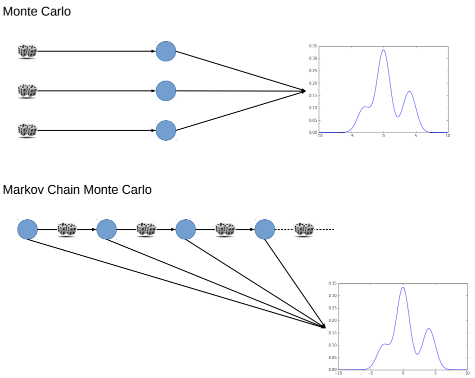
- modular structure
- simple python interfaces for getting started
- hierarchical models
- multilevel/multiindex MCMC methods

Markov Chain Monte-Carlo

- For the *forward problem* individual samples can be computed completely in parallel



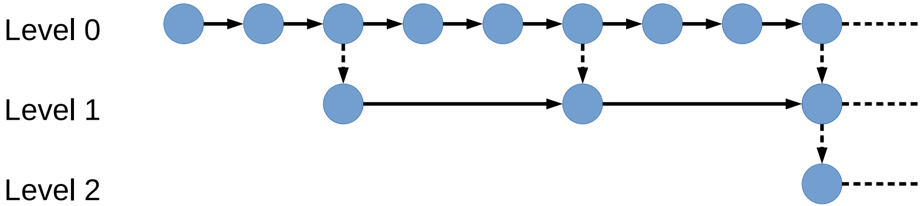
- For the *Bayesian inverse problem* each sample depends on the previous models → start several parallel Markov Chain



The multilevel idea

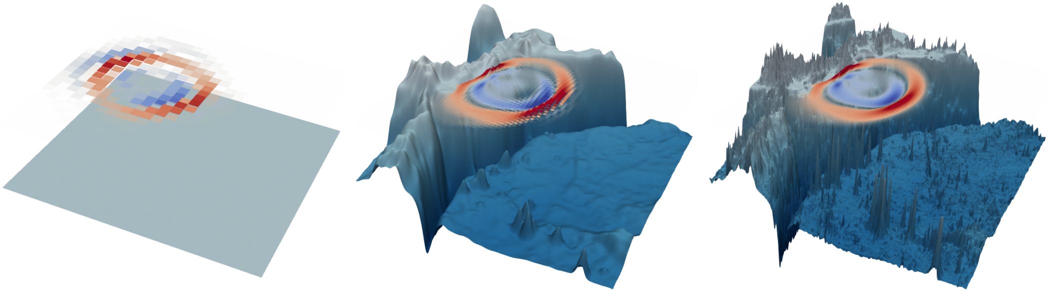
Telescoping sum of QOI like MLMC:

$$\mathbb{E}_{\nu^L}[Q_L] = \underbrace{\mathbb{E}_{\nu^0}[Q_0]}_{\text{Coarse approx.}} + \sum_{l=1}^{L} \underbrace{\left(\mathbb{E}_{\nu^l}[Q_l] - \mathbb{E}_{\nu^{l-1}}[Q_{l-1}]\right)}_{\text{Corrections}}.$$



The shallow water equations

Example: Tohoku tsunami originating in the Japan trench of 2011



https://www.noaa.gov/
https://www.gebco.net/
[Seelinger et al, accepted SC21]

Numerical Results

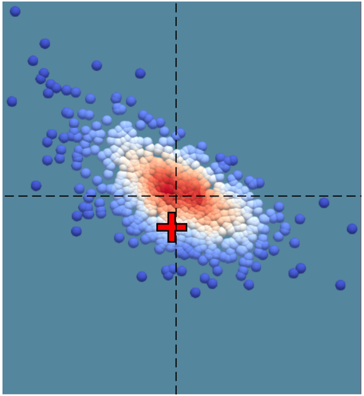


Figure: level 0

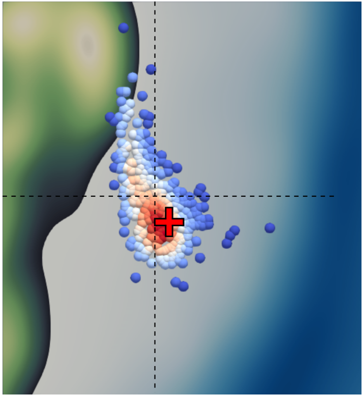


Figure: level 1

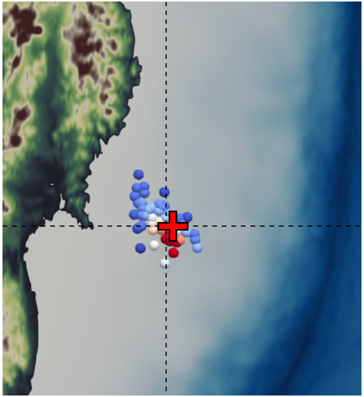
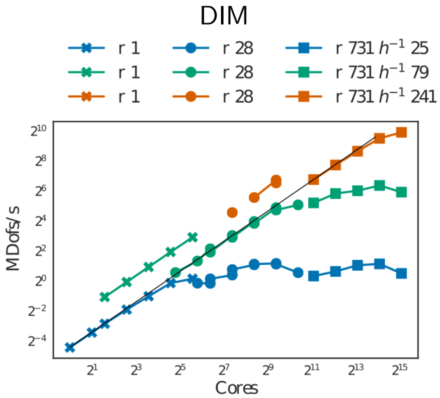
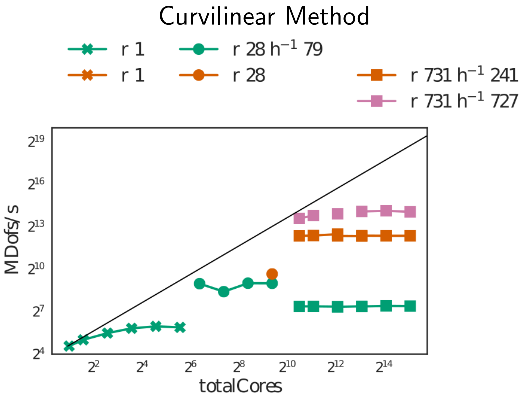


Figure: level 2

Hybrid Scaling on superMUC-NG

D. E. Carrier

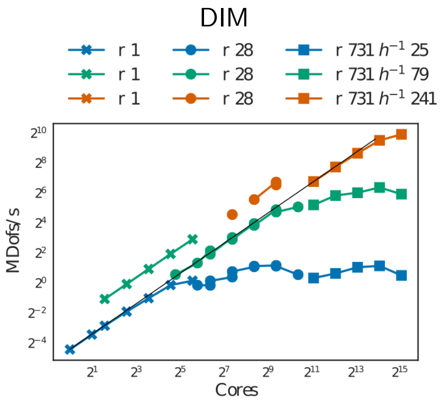


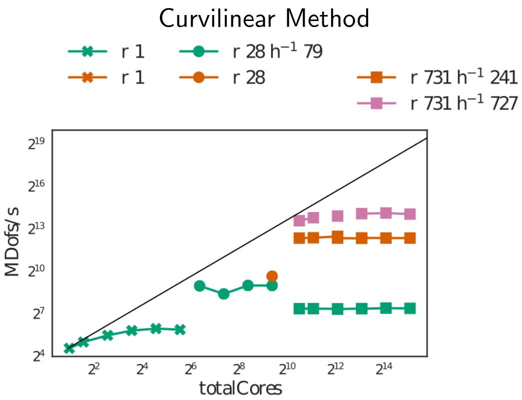


- DIM shows almost perfect weak and strong scaling.
- It reaches around 1 GDof/s on 731 nodes and 14 mio. elements.

Hybrid Scaling on superMUC-NG

D. E. Carrier





- Almost no strong scaling for Curvilinear method.
- It reaches around 16 GDof/s on 731 nodes and 384 mio. elements.

Challenges for Engine Development:

- lots of functionality to be tested, high effort for software integration.
- "multiple targets" for parallelisation and optimisation.
- equal number of cells does not lead to equal execution time.

Thus,

- in ExaHyPE we use a *task-based paradigm* for unpredictable work loads.
- tasks processing is build on a *produce-consumer pattern*. We assume volume operations are significantly more expensive than boundary operations (Prediction vs Riemann-solver).
- strategy for AMR: different granularity of AMR required by applications
- *communication-avoiding traversal scheme* that minimizes data transfer.
- *code generation* tailored to required PDE kernels.

Access to the Engine:

- snapshots of the engine, documentation, etc
  `www.exahype.org`
- webpage that comprises statistics, galleries, publication lists, etc.
  `exahype.eu`

References

[1] The ExaHyPE consortium. The ExaHyPE Guidebook. www.exahype.eu

[2] Reinarz et al. ExaHyPE: An engine for parallel dynamically adaptive simulations of wave problems. Computer Physics Communications. 2020.

[3] Tavelli et al. A simple diffuse interface approach on adaptive Cartesian grids for the linear elastic wave equations with complex topography. Journal of Computational Physics 386.

[4] Duru et al. A stable discontinuous Galerkin method for the perfectly matched layer for elastodynamics in first order form. 2019.

[5] Seelinger et al, High Performance Uncertainty Quantification with Parallelized Multilevel Markov Chain Monte Carlo. Accepted SC21