SeisSol and ExaHyPE: High-Order ADER-DG for Hyperbolic PDE Systems

Joint SeisSol and ExaHyPE User Workshop

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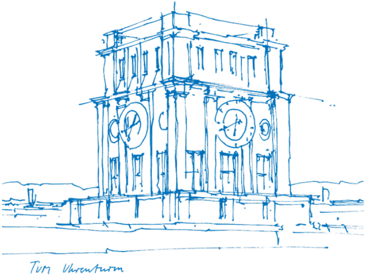


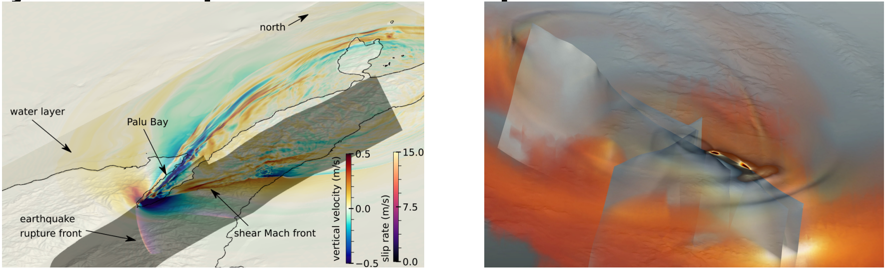
Part I

SeisSol – Extreme Scale Multi-Physics Earthquake Simulations

`http://www.seissol.org/` (all software open source)

Krenz et al. [3]: 3D acoustic-elastic coupling with gravity: the dynamics of the 2018 Palu, Sulawesi earthquake and tsunami.
Taufiqurrahman et al. [13]: Dynamics, interactions and delays of the 2019 Ridgecrest rupture sequence.
Uphoff et al. [6]: Extreme Scale Multi-Physics Simulations of the Tsunamigenic 2004 Sumatra Megathrust Earthquake.

Dynamic Rupture and Earthquake Simulation



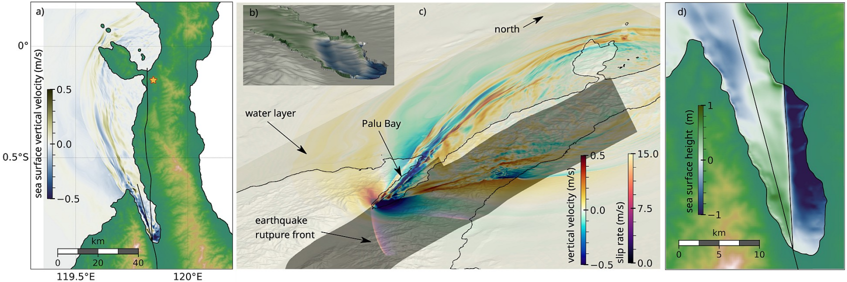
Dynamic rupture simulation with SeisSol: Sulawesi earthquake 2018 [3], Ridgecrest 2019 [13]

SeisSol – ADER-DG meets complex geometries: (www.seissol.org)

- adaptive tetrahedral meshes
  → complex geometries, heterogeneous media, multiphysics
- complicated fault systems with multiple branches
  → non-linear multiphysics dynamic rupture simulation
- ADER-DG: (adaptive) high-order discretisation in space and time
  → discontinuous Galerkin plus ADER (local) time stepping

ChEESE Pilot: Earthquake–Tsunami Simulation

Fully coupled acoustic-elastic simulations of submarine earthquakes & tsunami generation



3D coupled elastic-acoustic simulation of the 2018 Sulawesi earthquake (Krenz et al. [3], SC21)

Example: 2018 Sulawesi Earthquake and local tsunami in Palu Bay

- project ASCETE: follow-up on linked modeling of earthquake (dynamic rupture) simulation and subsequent shallow-water simulation, e.g. [14]
- ChEESE: fully-coupled simulation of elastic (solid earth) and acoustic (ocean) layer $\rightarrow$ coverage of complex 3D bathymetry

Seismic Wave Propagation with SeisSol

Elastic Wave Equations: (velocity-stress formulation)

$$q_t + Aq_x + Bq_y + Cq_z = 0$$

$$\text{with} \quad q = (\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}, \sigma_{23}, \sigma_{13}, u, v, w)^T \in \mathbb{R}^9$$

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\lambda - 2\mu & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\mu & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\mu \\ -\rho^{-1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\rho^{-1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\rho^{-1} & 0 & 0 & 0 \end{pmatrix} \qquad B = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\lambda - 2\mu & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\mu & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\mu \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\rho^{-1} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\rho^{-1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\rho^{-1} & 0 & 0 & 0 & 0 \end{pmatrix}$$

- high order discontinuous Galerkin discretisation
- **ADER-DG**: high approximation order in space and time
- additional features: local time stepping, high accuracy of earthquake faulting (full frictional sliding)

$\rightarrow$ Dumbser, Käser et al., esp. [10,11,12]

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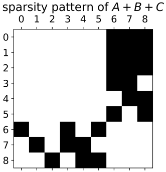

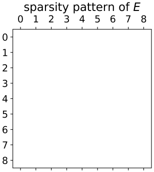

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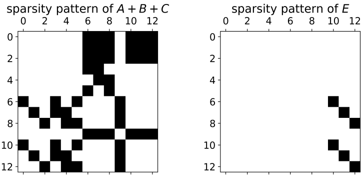
Seismic Wave Propagation with SeisSol

Poro-Elastic Wave Equations: (Wolf et al. [7], de la Puente et al. [9])

$$q_t + Aq_x + Bq_y + Cq_z = Eq$$

with $q = (\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}, \sigma_{23}, \sigma_{13}, u, v, w, p, u_f, v_f, w_f)^T \in \mathbb{R}^{13}$



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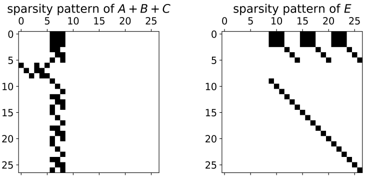
Seismic Wave Propagation with SeisSol

Visco-Elastic Wave Equations: (Uphoff et al. [4], Käser et al. [12])

$$q_t + Aq_x + Bq_y + Cq_z = Eq$$

with $q = (\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}, \sigma_{23}, \sigma_{13}, u, v, w, \zeta_{11}^1, \ldots, \zeta_3^3)^T \in \mathbb{R}^{9+6L}$



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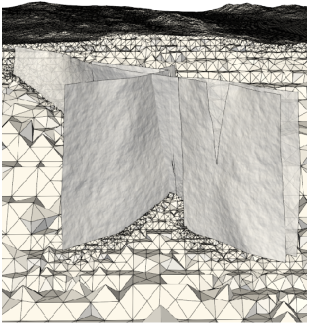
DG on Tetrahedral Meshes

Weak Form of the elastic wave equations:

$$\int_{T_k} q_t \phi_m \, d\vec{x} + \int_{T_k} (Aq_x + Bq_y + Cq_z)\phi_m \, d\vec{x} = 0$$

Apply chain rule and divergence theorem:

$$\int_{T_k} q_t \phi_m \, d\vec{x} = \int_{T_k} Aq(\phi_m)_x + Bq(\phi_m)_y + Cq(\phi_m)_z \, d\vec{x} - \int_{\partial T_k} F\phi_m \, d\vec{s}$$



Further choices:

- modal basis ϕ_m; ϕ_m orthogonal to obtain diagonal mass matrix
- hierachical (w.r.t polynomial degree) basis ϕ_m, leads to staircase pattern in stiffness matrices
- exact Riemann solver for linear flux F
- ADER time stepping ("Arbitrary high-order DERivatives")

SeisSol Numerics in a Nutshell – ADER-DG

Update scheme

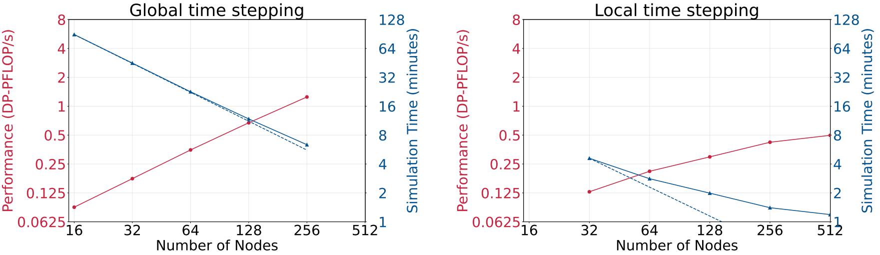
$$
\begin{aligned}
Q_k^{n+1} = Q_k - \frac{|S_k|}{|J_k|} M^{-1} \Bigg(& \sum_{i=1}^{4} F^{-,i} I(t^n, t^{n+1}, Q_k^n) N_{k,i} A_k^+ N_{k,i}^{-1} \\
& + \sum_{i=1}^{4} F^{+,i,j,h} I(t^n, t^{n+1}, Q_{k(i)}^n) N_{k,i} A_{k(i)}^- N_{k,i}^{-1} \Bigg) \\
& + M^{-1} K^{\xi} I(t^n, t^{n+1}, Q_k^n) A_k^* \\
& + M^{-1} K^{\eta} I(t^n, t^{n+1}, Q_k^n) B_k^* \\
& + M^{-1} K^{\zeta} I(t^n, t^{n+1}, Q_k^n) C_k^*
\end{aligned}
$$

Cauchy Kovalewski

$$
I(t^n, t^{n+1}, Q_k^n) = \sum_{j=0}^{J} \frac{(t^{n+1} - t^n)^{j+1}}{(j+1)!} \frac{\partial^j}{\partial t^j} Q_k(t^n)
$$

$$
(Q_k)_t = -M^{-1} \left((K^{\xi})^T Q_k A_k^* + (K^{\eta})^T Q_k B_k^* + (K^{\zeta})^T Q_k C_k^* \right)
$$

Scaling and Performance on Frontier (GPU)



Strong scaling and performance on Frontier for the Kahramanmaras scenario (mesh with 175 million elements) – comparing global (left) and local(right) time stepping.

Performance vs. time to solution of Local Time Stepping on Frontier

- on 16–512 nodes (4 AMD Instinct MI250X GPUs per node)
- $> 2\times$ performance advantage of GTS
- $\sim 5\times$ improvement (on 32 nodes) in solution time due to LTS

Part II

ExaHyPE – Building an Exascale Hyperbolic PDE Engine

"They are skating to
where the puck will be . . . "
(David Keyes)

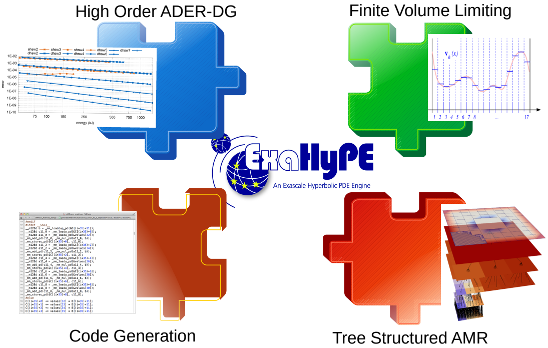
ExaHyPE
An Exascale Hyperbolic PDE Engine

Wayne Gretzky (image source: Wikipedia)

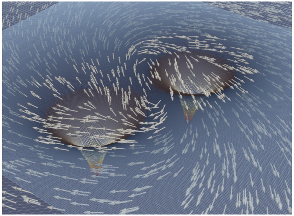
Towards an Exascale Hyperbolic PDE Engine

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

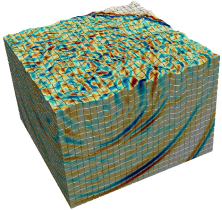
- enable medium-sized interdisciplinary research teams to realise extreme-scale simulations of grand challenges within one year
- focus on hyperbolic conservation laws and high-order DG
- fixed numerics and mesh infrastructure, but **stay flexible w.r.t. PDE**



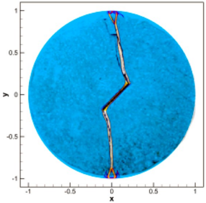
Applications with the ExaHyPE Engine



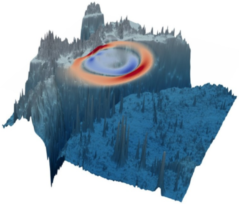
relativistic astrophysics [27,34]



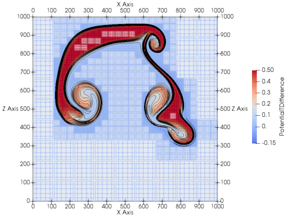
seismic waves [17,18,19]



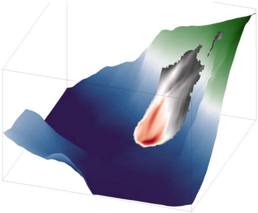
crack propagation [29,32]



shallow water [28,23]



cloud formation [30]

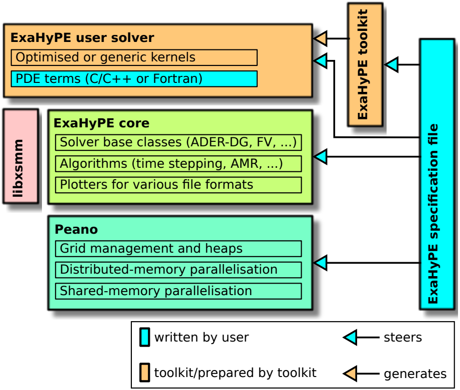


landslides

ExaHyPE's Software Architecture

Solve systems of 1st-order hyperbolic PDEs of the form:

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



Using the ExaHyPE Toolkit:

1. create a specification file that defines the domain, PDE system, required architecture, parallelisation, etc.
2. ExaHyPE toolkit creates glue code, application-specific template classes and core routines (tailored to application and architecture)
3. implement the application classes with PDE- and scenario-specific methods:
   - `flux(...)`, `ncp(...)`, ... for PDE terms (conservative fluxes, non-conservative products, etc.)
   - `eigenvalues(...)` to compute eigenvalues (for Riemann solvers)
   - `boundaryValues(...)`, etc.

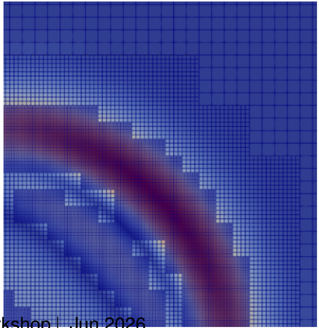
ADER-DG with Finite Volume Limiting

Disc. Galerkin with Space-Time Basis Functions: (Zanotti et al. [33])

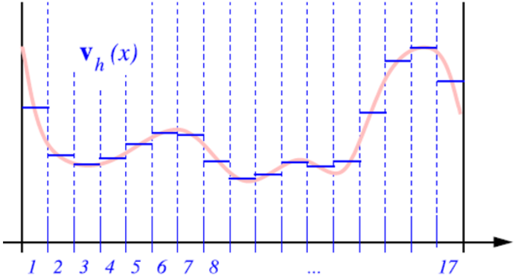
- formulated for general hyperblic PDE system: $u_t + \nabla \cdot F(u) = 0$
- integrate over space-time control volume $T_k \times [t_n, t_{n+1}]$ and integrate by parts:

$$\int_{t_n}^{t_{n+1}} \int_{T_k} \phi_m \frac{\partial u_h}{\partial t} dxdt + \int_{t_n}^{t_{n+1}} \int_{\partial T_k} \phi_m F(u_h)\, d\vec{S}dt - \int_{t_n}^{t_{n+1}} \int_{\partial T_k} \nabla \phi_m \cdot F(u_h) dxdt = 0$$

- element-local fixpoint scheme to solve space-time problem (“Picard loop”)
- generalized Riemann solver to obtain $F(\cdot)$ on boundaries
- Riemann solver flexible: Rusanov, Osher-type, HLL-type, custom, ...
- on tree-structured adaptive Cartesian meshes



Finite-Volume Limiting



- perform non-limited DG step (space-time prediction & correction)
- check DG-solution candidate for physical and numerical feasibilty
- flag cells as “troubled”, if solution not feasible
- re-compute solution via Finite-Volume scheme
  on a $(2p+1) \times (2p+1)$ patch (with the same time step)

SeisSol Publications

[1] A. Breuer, A. Heinecke, M. Bader: Petascale local time stepping for the ADER-DG Finite Element method. Proc. IPDPS16.

[2] R. Dorozhinskii, G. Brito Gadeschi, M. Bader: *Fused GEMMs towards an efficient GPU implementation of the ADER-DG method in SeisSol.* Concurr. & Comput.: Pract. & Exp., 2024.

[3] L. Krenz, C. Uphoff, T. Ulrich, A.-A. Gabriel, L.S. Abrahams, E.M. Dunham, M. Bader: *3D acoustic-elastic coupling with gravity: the dynamics of the 2018 Palu, Sulawesi earthquake and tsunami.* SC21.

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[5] C. Uphoff, M. Bader: *Yet Another Tensor Toolbox for discontinuous Galerkin methods and other applications*. ACM TOMS 46(4). `https://doi.org/10.1145/3406835`.

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[7] S. Wolf, M. Galis, C. Uphoff, A.A. Gabriel, P. Moczo, D. Gregor, M. Bader: *An efficient ADER-DG local time stepping scheme for 3D HPC simulation of seismic waves in poroelastic media.* J. Comput. Phys. 455, 2022.

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