Wave propagation in anisotropic and poroelastic media using high order ADER-DG

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SeisSol: ADER-DG for earthquake dynamics

SeisSol (`https://seissol.org`) is a well-established simulation software for earthquakes source dynamics and seismic wave propagation. SeisSol solves the hyperbolic PDE

$$\partial_t q + A\partial_x q + B\partial_y q + C\partial_z q = Eq. \tag{1}$$

We are able to simulate realistic earthquake scenarios for (visco)elastic materials with optional plastic deformation. Dynamic rupture is used to incorporate physics based source dynamics. Heterogeneous materials and topography are supported out-of-the-box [2].

Discontinuous Galerkin discretisation

We use the Discontinuous Galerkin (DG) method on unstructured tetrahedral grids. With Arbitrary DERivative (ADER) time stepping we achieve high order in space and time.
We predict the solution locally in each element, and then correct the solution using numerical fluxes across element boundaries. The space-time prediction is usually done via a Taylor series, where we obtain the time derivatives from the Cauchy-Kovalevski procedure.
The numerical scheme results in a sequence of small matrix-matrix multiplication, e.g:

$$\begin{aligned}\partial_t^{j+1} Q_k^n = M^{-1}\Big[&(K^\xi)^T \left(\partial_t^j Q_k^n\right) A_k^* \\ &+ (K^\eta)^T \left(\partial_t^j Q_k^n\right) B_k^* + (K^\zeta)^T \left(\partial_t^j Q_k^n\right) C_k^*\Big].\end{aligned} \tag{2}$$

In the case of poroelasticity, we encounter a stiff source term. The approach from eq. (2) then suffers from a severe time step restriction to ensure stability.
We therefore expand the solution using temporal ansatz functions:

$$Q_k(x,y,z,t) = Q_{klm}\phi_l(x,y,z)\chi_m(t). \tag{3}$$

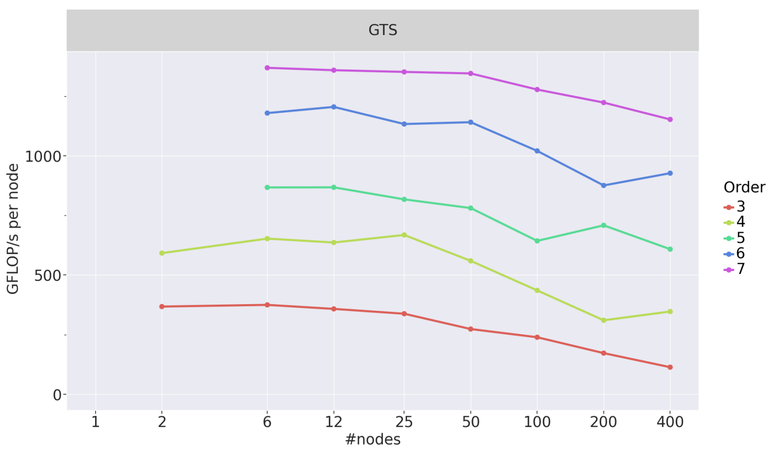
If we plug this identity into the ADER-DG formalism, we obtain the linear system:

$$\begin{aligned}Q_{mou} - \hat{S}_{uk}\Big(&A^*_{oq}\hat{K}^\xi_{ml}Q_{lqk} + B^*_{oq}\hat{K}^\eta_{ml}Q_{lqk} \\ &+ C^*_{oq}\hat{K}^\zeta_{ml}Q_{lqk} + E^*_{oq}Q_{mqk}\Big) \\ &= \hat{w}_u Q^0_{mo}.\end{aligned} \tag{4}$$

With this space-time ansatz we are able to integrate a broader class of PDEs with reasonable time steps.
We use the code generator `YATeTo` to map these expressions to a sequence of small GEMMs. Architecture specific backends, such as e.g. `libxsmm`, give excellent node-level performance.

Parallelisation strategy

With typically over a billion degrees of freedom, the equations can only be solved parallel. We use a hybrid MPI+OpenMP parallelization. Inter node parallelism is based on mesh partitioning. On the node level we use OpenMP to update the elements in a parallel manner. SeisSol is originally a CPU code, but a GPU port is work in progress. The space time predictor is not yet ported.



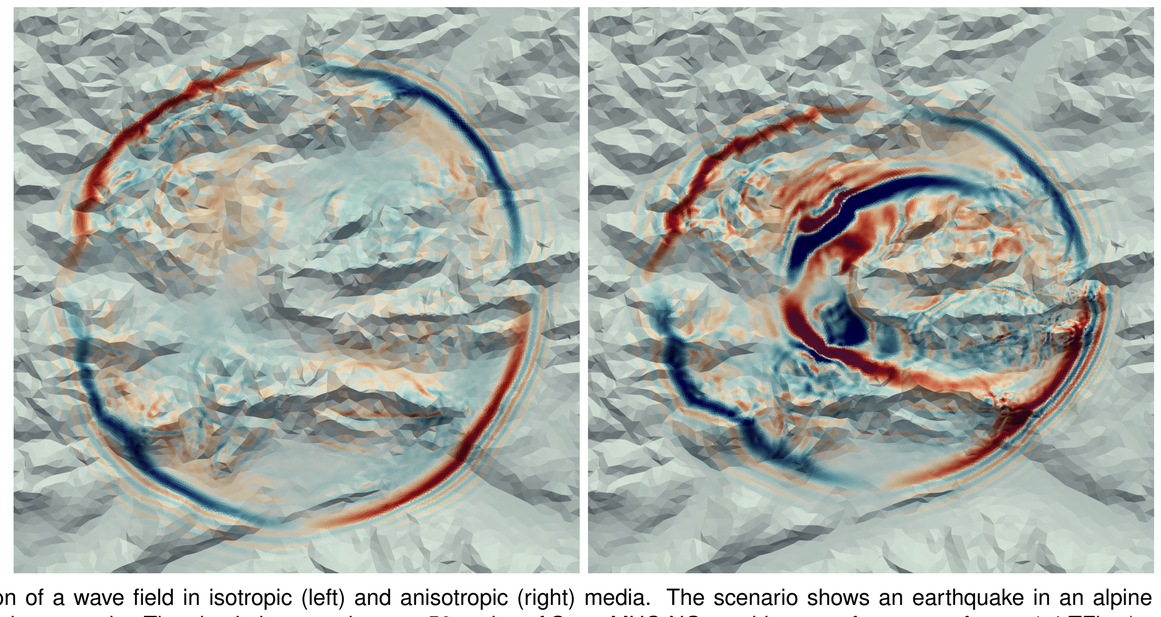
Parallel efficiency for a medium sized test case (7.3M elements) with global time stepping. For this simulation we already used the new space time predictor kernel. Experiments were carried out on SuperMUC-NG.

Extension to Triclinic anisotropic elasticity

Motivation
In anisotropic media, the wave speeds depend on the direction of propagation. Such effects can stem from cracks in the medium or layered sediments.

Necessary changes
Instead of 3 (for isotropic elastic media), now up to 22 different material parameters are needed to describe the triclinic anisotropic behaviour. The Jacobians A, B, C are more densely populated. The Riemann Solver needs an eigendecomposition of these matrices. Since for the anisotropic case analytic expressions are not available any more, we use a numerical solver from `eigen3` to compute the eigenvalue decomposition.
The computational overhead is negligible since the decomposition is only done once in the setup phase and then stored.

Results
We achieve similar performance as for the isotropic case: 1.4 TFlop/s per node with global time stepping and 1.0 TFlop/s per node with local time stepping on SuperMUC-NG (2xIntel Skylake Xeon Platinum 8174, 96 GB RAM, LINPACK: 3.0 TFlop/s per node). The increased number of material parameters causes a higher memory consumption, but performance stays compute bound.



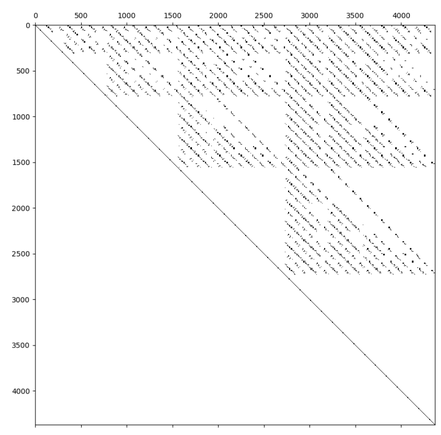
Comparison of a wave field in isotropic (left) and anisotropic (right) media. The scenario shows an earthquake in an alpine region with complicated topography. The simulation was done on 50 nodes of SuperMUC-NG reaching a performance of up to 1.4 TFlop/s per node.

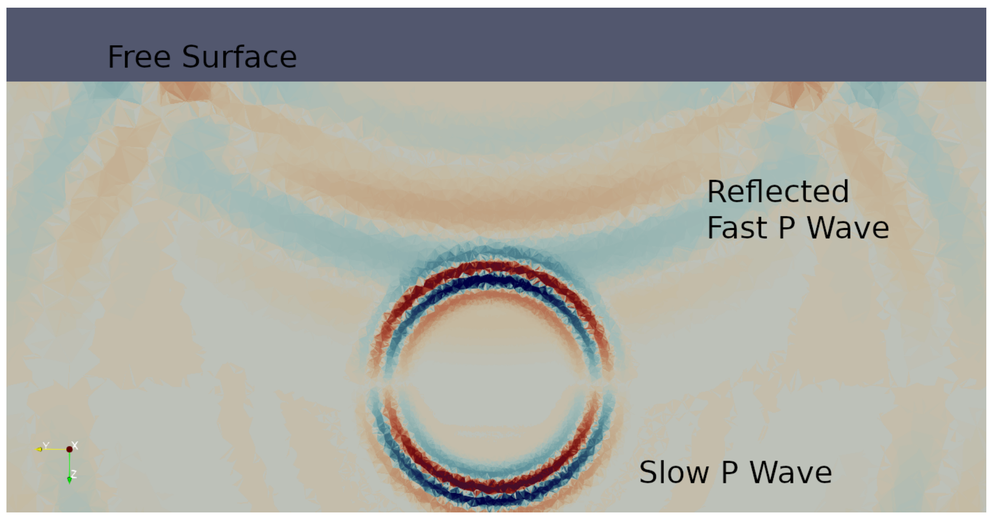
Extension to Poroelasticity - ADER-DG with a stiff source term

Motivation
In the context of geothermal energy, the Earth has to be modelled as porous, fluid-filled medium. Therefore, we use Biot's theory of poroelastic media [3] in order to investigate induced earthquakes.

Necessary changes
In addition to the velocities and stresses in the solid, we introduce the fluid velocities and pressure as unknowns to eq. (1). The source term Eq is used to model the coupling between solid and fluid phase.
The resulting system of PDEs is stiff. Therefore the existing time stepping scheme becomes unstable.
We introduce a space-time predictor to overcome the stability issues. As a consequence, the element-local update scheme consists of the solution of a linear system with a few thousand unknowns. Again, we can map the solution procedure to a sequence of small GEMMs to achieve high performance.

Results
We are validating the new scheme against various reference solutions. A convergence test verifies that the high order is obtained. Additional tests cover point sources, material heterogeneities and the free surface boundary condition. To solve the element-local system, our approach needs 311 operations per DOF to compute one time step for one cell when using the scheme of order 6. With the naive approach, i.e. to solve the system with a precomputed LU decomposition, the backward substitution step alone would need 8740 operations per DOF. By using the optimized algorithm we reduced the workload to $\sim 3.6\%$ of the original.
The new compute kernel reaches a node level performance of up to 1.3 TFlop/s on SuperMUC-NG, which is 40% of the peak performance. With local time stepping the node level performance decreases, but overall time to solution still benefits.





Left: Sparsity pattern of the element-local matrix for convergence order 6. If the indices are correctly permuted we obtain the system in upper block diagonal form. We can use block wise back substitution solve the system. Right: Snapshot of the wave field excited by an explosive point source in a poroelastic medium. One can see the reflected fast P wave and the slow P wave, which is a distinct feature of poroelastic media.

Acknowledgements

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References

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