An Efficient ADER-DG Scheme for Simulation of Seismic Waves in Poroelastic Media

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Summary

The equation of motion for poroelastic media based on Biot's theory contains a stiff reactive term that poses a key computational challenge for numerical methods. We present an efficient **ADER-DG scheme (discontinuous Galerkin scheme with Arbitrary high-order DERivative time stepping)** for solving problems with the stiff term utilizing a novel block-wise back-substitution algorithm. For polynomials of degree 6, the number of floating-point operations is reduced by a factor of 25 compared to the standard LU decomposition. Additionally, the block-wise back-substitution is mapped to a sequence of small matrix-matrix multiplications, for which code generators are available to generate highly optimized code. This way, we achieve excellent node-level performance.
We verify the new scheme thoroughly against (semi)analytical or numerical reference solutions in canonical problems of increasing complexity using a point source. Additionally, by utilizing a clustered local time-stepping scheme, time to solution is reduced by a factor of 6 to 10 compared to the global time stepping. Performance analysis on the SuperMUC-NG supercomputer demonstrates high computational efficiency of our implementation and its potential for extreme-scale simulations.

ADER-DG Scheme

Governing equation for wave propagation in a **poroelastic medium** in matrix-vector form:

$$\frac{\partial q}{\partial t} + A\frac{\partial q}{\partial x} + B\frac{\partial q}{\partial y} + C\frac{\partial q}{\partial z} = E.q$$

q is the vector of unknowns consisting of six stress components, three particle velocity components, pore pressure and three relative fluid velocities:

$$q = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{yz}, \sigma_{xz}, u, v, w, p, u_f, v_f, w_f)^T$$

$E.q$ is the viscous dissipation term and presents **the challenging stiff term**

Matrices A, B, C and E contain material properties and have specific sparsity patterns (see Fig 1)

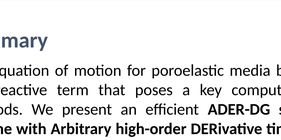


Figure 1
Sparsity pattern of matrix
Left $A + B + C$
Right E

Time integration is performed using a **predictor-corrector scheme**, in which the locally predicted solution is corrected using numerical fluxes. The Cauchy-Kovalewski procedure, used as the predictor for (visco-)elastic media, is unstable in the presence of the stiff term. Therefore, we adopt the **space-time predictor** proposed by de la Puente *et al.*, 2008. The idea is to express the solution on the reference element in space and time using a polynomial basis functions

$$Q_p(\xi,\eta,\zeta,\tau) = Q_{pls}.\chi_l(\tau).\phi_s(\xi,\eta,\zeta)$$

Following the derivation by de la Puente *et al.*, 2008, the system of equations for Q_{pls} can be written in the form

$$Y_{pkrqls}Q_{pls} = R_{pkr}$$

The operator Y_{pkrqls} and the right-hand side r_{pkr} are

$$Y_{pkrqls} = \delta_{pq}W_{rs}M_{kl} - \delta_{pq}K^{\tau}_{rs}M_{kl} - E^{*}_{pq}S_{rs}M_{kl} + \sum_{j=1}^{3} A^{j*}_{pq}S_{rs}K^{j}_{kl}$$

$$R_{pkr} = \delta_{pq}w_r M_{kl}Q^{0}_{ql}$$

where

$$W_{rs} = \chi_r(1)\chi_s(1)$$
$$w_r = \chi_r(0)$$
$$S_{rs} = \int_0^1 \chi_r\chi_s d\tau$$
$$K^{\tau}_{rs} = \int_0^1 \frac{\partial\chi_r}{\partial\tau}\chi_s d\tau$$
$$M_{kl} = \int \phi_k\phi_l dV$$
$$K^{\alpha}_{kl} = \int \phi_k \frac{\partial\phi_l}{\partial\alpha} dV \qquad \alpha \in \{\xi,\eta,\zeta\} \text{ or } \{1,2,3\}$$

and matrices A^{j*} are Jacobian matrices composed from matrices A, B and C. See Wolf *et al.*, 2022 for detailed derivation and discussion

We present an **efficient ADER-DG scheme** for simulating **seismic waves in poroelastic media**

Our **novel algorithm** for treating the **stiff source term reduces the number of operations by a factor of 25** compared to the standard LU decomposition algorithm for basis functions of degree 6

Our **implementation in SeisSol** (www.seissol.org) **reduces the time to solution by a factor of about 10** compared to an ideally performing LU decomposition

PrePrint

Wolf, Galis, Uphoff, Gabriel, Moczo, Gregor, Bader, 2022.
An Efficient ADER-DG Local Time Stepping Scheme for 3D HPC Simulation of Seismic Waves in Poroelastic Media,
Journal of Computational Physics, 455.
doi: 10.1016/j.jcp.2021.110886

The Novel Block-Wise Back-Substitution Algorithm

By **unrolling the multi-indices** *pkr* and *qls* to *i* and *j*, respectively, the system $Y_{pkrqls}Q_{pls} = R_{pkr}$ can be written in **standard matrix form**, $Ax = b$

Choosing *k/l* as the slowest and *r/s* as the fastest-running indices leads to a **specific block-structure of the system matrix** (see Fig 2).

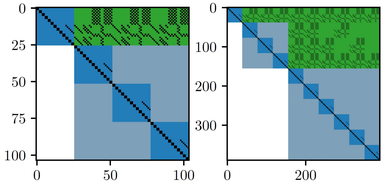


Figure 2
Sparsity pattern of the system matrix for basis functions with the maximum degree 1 (*left*) and 2 (*right*)

blocks: only zeros
diagonal blue blocks:
light blue: only zeros
dark blue: upper block-triangular
green blocks: recurring sparsity pattern

Our **novel algorithm** (see Fig 3) **utilizes**

- the block-wise back-substitution exploiting the block-triangular structure of the system matrix
- the upper triangular sparsity pattern of the matrix E^*
- the internal structure of blue and green blocks
- tensor operations

```
b ← Q^0 ∘ (S^{-1} w);
for n ← N downto 0 do
    // dark and light-blue blocks together
    m ← (B_{n-1}, B_n];
    for p ← Q downto 1 do
        Q_{pm:} ← b_{pm:} · (Z − E*_{pp} I)^{-T} ;
        for o ← 1 to p − 1 do
            b_{om:} ← b_{om:} + G_{op} · Q_{pm:} ;
        end
    end
    // green blocks
    if n > 0 then
        b ← b − A* ×_1 Q_{:m:} ×_2 K̂^ξ_{:m} ;
        b ← b − B* ×_1 Q_{:m:} ×_2 K̂^η_{:m};
        b ← b − C* ×_1 Q_{:m:} ×_2 K̂^ζ_{:m};
    end
end
```

Figure 3 u
The scheme of our novel algorithm (Algorithm 3 in Wolf *et al.*, 2022)

Performance

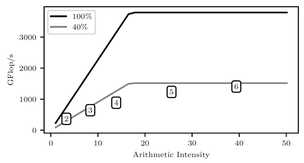
Advantages

- **lower number of FLOPs** compared to standard LU decomposition (see Tab 1)
- **lower memory requirements** than standard LU decomposition (see Tab 1)
- because the algorithm is defined via tensor operations, **the code generator YATeTo** (Uphoff *et al.*, 2020) can be used to **translate/map the tensor operations to small matrix-matrix multiplications**, for which **highly optimized architecture-specific code** generators are available
- **time to solution** with our SeisSol implementation is **about 10 times shorter** than with ideally performing LU decomposition
- the algorithm can be combined with **local time stepping** – for example, for LOHp test, the time to solution is 6 to 10 times shorter than with global time stepping depending on the number of used nodes and convergence order

Table 1 Comparison of number of floating-point operations and memory requirements of standard LU decomposition (LU) and our optimized algorithm 3 for the space-time predictor approach (STP). [*N* – maximum degree of basis functions, *n* – number of unknowns]

N	*n*	FLOPs			storage		
		LU	STP	reduction	LU [MB]	STP [MB]	reduction
4	2275	1.04×10^7	7.13×10^5	**14.5**	39.5	6.4×10^-3	**6179**
5	4368	3.82×10^7	1.94×10^6	**19.7**	145.6	7.5×10^-3	**19453**
6	7644	1.17×10^8	4.72×10^6	**24.8**	445.9	8.8×10^-3	**50816**

Figure 4 u
The roofline model shows that our implementation in SeisSol performs at approx. 40% of the theoretical peak performance of a single node of SuperMUC-NG supercomputer. The numbers in squares depict the maximum degree of basis functions.



Numerical Tests - Verification

Convergence test

- planar wave as the initial condition
- analytical reference solution
- expected convergence rate achieved for all unknowns

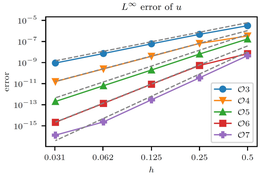


Figure 5 u
Convergence plot for particle velocity *u*. Dashed gray lines depict the expected convergence rates.

Point source in homogenous space

- explosive point source at (0,0,0)
- semi-analytical reference solution (Karpfinger *et al.*, 2009)
- excellent agreement for inviscid as well as viscous cases

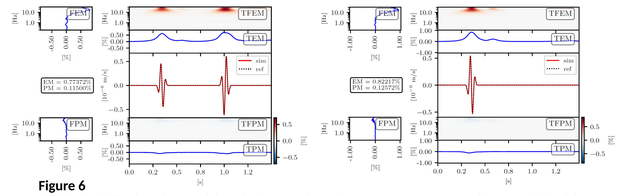


Figure 6
Detailed misfit plots for particle velocity *u* at location (575m,575m,575m) for materials with the pore space filled by inviscid fluid (*left*) and viscous fluid (*right*).

Boundary conditions

- explosive point source
- semi-analytical reference solution (gar6more3D by Diaz *et al.*, 2008)
- only inviscid case (due to limitations of the reference solution)
- excellent agreement for free surface boundary condition and internal interface

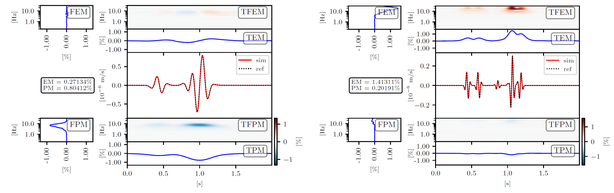


Figure 7
Detailed misfit plots for particle velocity *u* in inviscid case. *Left*: Free-surface boundary condition – receiver at a shallow depth (due to limitations of the reference solution). *Right*: Internal interface – receiver 500m behind the interface captures transmitted waves.

Layer over halfspace (LOHp)

- explosive line source
- 2D finite difference reference solution (Gregor *et al.*, 2021)
- important **for most practical applications**:
  - **excellent agreement** for solid particle velocities with standard resolution
- important **for specific applications**:
  - if the relative fluid velocities must be calculated at or very close to the free surface or an internal interface, **finer resolution is necessary** in both methods

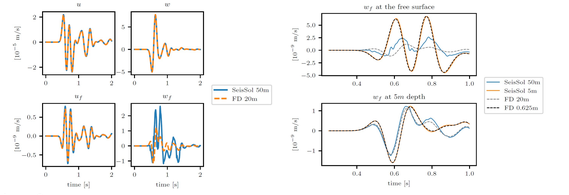


Figure 8
Comparison of solid particle velocities (*u* and *w*) and relative fluid velocities (u_f and w_f) in the LOHp model. *Left*: The receiver at the free surface shows excellent agreement for solid particle velocities using standard resolution. *Right*: Illustration of the small-scale effect of the diffusive slow P-wave near the free surface using fine resolution.

References

Diaz, Ezziani, 2008. „Analytical Solution for Wave Propagation in Stratified Poroelastic Medium. Part II: ...", arXiv:0807.4067

Gregor, Moczo, Kristek, Mesgouez, et al., 2021. „Subcell-resolution finite-difference modelling of seismic ...", GJI 224

Karpfinger, Muller, Gurevich, 2009. „Green's functions and radiation patterns in poroelastic solids revisited", GJI 178

de la Puente, Dumbser, Käser, Igel, 2008. „Discontinuous Galerkin methods for wave propagation ... ", Geophysics 73

Uphoff, Bader, 2020. „Yet Another Tensor Toolbox for ...", ACM Transactions on Mathematical Software 46

Misfits used for quantitative comparison of the solutions:

Kristekova, Kristek, Moczo, Day, 2006. „Misfit Criteria for Quantitative Comparison of Seismograms", BSSA 96

Kristekova, Kristek, Moczo, 2009. „Time-frequency misfit and goodness-of-fit criteria for quantitative ...", GJI 178