Advanced Material Models for Seismic Simulations using ADER-DG

SIAM GS21

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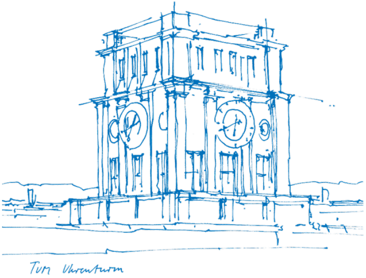
21st June, 2021

The research leading to these results has received funding from European Union Horizon 2020 research and innovation program (ENERXICO, grant agreement No. 828947).



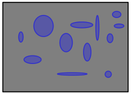
Motivation

ENERXICO

Seismic wave propagation for applications in the energy sector

- Not just elasticity
- Cracked or damaged rock
- Interaction with a fluid phase

⇒ anisotropic and poroelastic materials



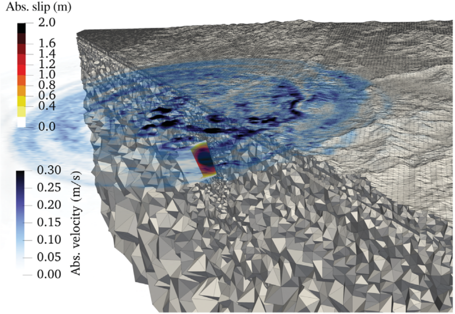
In particular we are interested in the interplay of induced earthquake rupture, wave propagation, complex topography and poroelastic effects.

Earthquake simulations

Use SeisSol to solve the elastic wave equation:

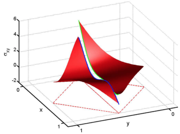
- $\partial_t q + A\partial_x q + B\partial_y q + C\partial_z q = 0$
- q collects stresses and velocities

(Palgunadi et al. 2020): "Dynamic Fault Interaction during a Fluid-Injection-Induced Earthquake: The 2017 Mw 5.5 Pohang Event"



Discontinuous Galerkin method

- Discretize Ω in tetrahedrons
- Expand the solution in terms of polynomials $q_p(t, \vec{x}) = Q_{pl}(t)\phi_l(\vec{x})$.
- Multiply the PDE with an element local test function ψ and integrate by parts
- Use numerical fluxes to exchange informations between elements.



High-Order time stepping

Can be combined with time stepping like ~~Runge-Kutta or~~ Arbitrary DERivatives ansatz.

- Expand solution in time as a Taylor series around t^n to predict solution
- Use space derivatives at time t^n to get the time derivatives with the Cauchy-Kowalevski procedure
- Use fluxes to correct the solution

$\Rightarrow$ Achieve same convergence order in space *and* time

HPC Optimizations

Parallelization

- Element local discretization with DG
- Mesh partitioning based on workload estimate
- Exchange values at partion boundaries

Node-level performance

- Update scheme is a sequence of tensor contractions
- Use `YATeTo`[1] to map the tensor operations to GEMMs ($C = \alpha AB + \beta C$)
- Use architecture specific backends (like `libxsmm`) for optimized code

[1] (Uphoff and Bader 2020)

Model extensions – Anisotropy

Anisotropic material: directional dependent material behaviour
In seismology: layered or cracked media
For SeisSol: Extend work from (Puente, Käser, et al. 2007)

Necessary changes:

- Jacobian matrices A, B and C more densely populated.
- Flux solver needs an eigendecomposition: switch from analytic expression to numerical solver
- Wave speeds depend on the direction: switch from single evaluation to sampling
- Free surface boundary condition: Solve an inverse Riemann Problem

Anisotropy – application example

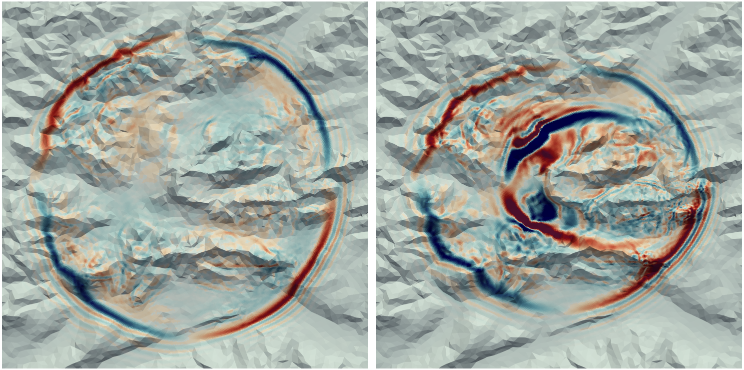


Figure: Vertical velocity field after 3 s, left: isotropic material, right: anisotropic material

Model extensions – Poroelasticity

Poroelastic material: porous elastic medium, filled with a fluid
In seismology: georeservoirs

Necessary changes:

- q now contains fluid pressure p and fluid velocities as additional quantities
- Coupling between fluid and solid phase for low frequencies:
  $\partial_t q + A\partial_x q + B\partial_y q + C\partial_z q = \boxed{Eq}$
- System of PDEs is stiff!
- ~~reduce time-step or~~ use (locally) implicit scheme

Poroelasticity – Space time predictor

Before: Expand the solution from t^n as Taylor series in time

Now: $q_p(t, \vec{x}) = Q_{pts}\phi_l(\vec{x})\chi_s(t)$ (Puente, Dumbser, et al. 2008)

- Plug this into the discretization to obtain a linear system of equations.
- For order 6 this has 4368 unknows.
- We have to solve this system for every element and every timestep.
- Standard approach: precompute LU decomposition, do backsubstitution
  $\Rightarrow$ 38.2 MFLOP for the backsubstitution only

Poroelasticity – System of equations

Solve a linear equation in tensorial form: $O_{pksqlt}Q_{qlt} = b_{pks}$:

$$
\begin{aligned}
&\delta_{pq} \left\langle \chi_s(1)\phi_k, \chi_t(1)\phi_l \right\rangle Q_{qlt} - \delta_{pq} \left[\frac{\partial}{\partial \tau}\chi_s\phi_k, \chi_t\phi_l \right] Q_{qlt} \\
&+ A^*_{pq} \left[\chi_s\phi_k, \chi_t \frac{\partial}{\partial \xi}\phi_l \right] Q_{qlt} + B^*_{pq} \left[\chi_s\phi_k, \chi_s \frac{\partial}{\partial \eta}\phi_l \right] Q_{qlt} \\
&+ C^*_{pq} \left[\chi_s\phi_k, \chi_t \frac{\partial}{\partial \zeta}\phi_l \right] Q_{qlt} - E^*_{pq} \left[\chi_s\phi_k, \chi_s\phi_l \right] Q_{qlt} \\
&= \delta_{pm} \left\langle \chi_s(0)\phi_k, \phi_n \right\rangle Q^0_{mn}.
\end{aligned}
$$

Poroelasticity – Examine the system more closely

Unroll *pks* and *qlt* to linear indices:

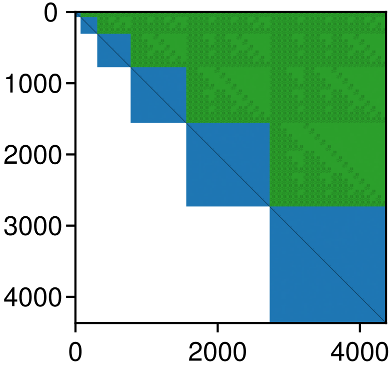


Figure: Sparsity pattern of the system matrix, if unrolled correctly

Poroelasticity – Improved solver

- System is already in upper triangluar form, but with blocks of size $\mathcal{O} \times \mathcal{O}$ on the diagonal.
- Use blockwise backsubstitution to solve the system.
  $\Rightarrow$ 1.94 MFLOP
- This is only 4 % of the original workload.
- Blockwise backsubstitution can be mapped to GEMMs with `YATeTo` for high performance

Poroelasticity – Results

- Convergence test ✓
- Various benchmarks against analytic solutions ✓
- LOHp ✓

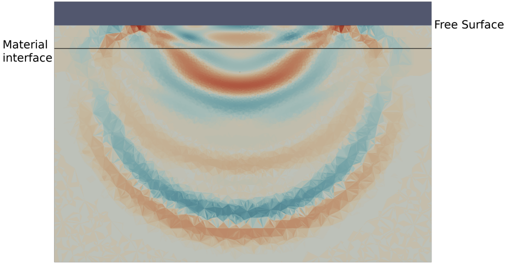


Figure: Layer over halfspace scenario with poroelastic materials. Vertical velocity after 1 s.

Poroelasticity – Parallel efficiency

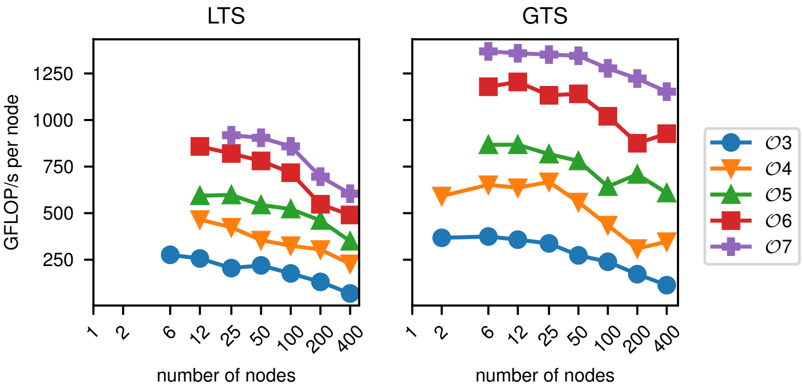


Figure: Parallel efficiency for a mesh with 7.33 million elements. We see good scaling until 100.000 elements per node.

Conclusion

- Successfully added anisotropic material behaviour to SeisSol
- Extension to poroelastic materials is work-in-progress, with promising results

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Algorithm design for the inversion procedure in collaboration with Carsten Uphoff and Martin Galis.

Backup Slide Equations

Weak formulation of the PDE in 1D:

$$\int_T \partial_t q \cdot \phi \mathrm{d}x - \int_T Aq\partial_x \phi \mathrm{d}x + \int_{\partial T} \phi Aq \cdot n \mathrm{d}s = \int_T Eq\phi \mathrm{d}x$$

Semidiscrete form:

$$\begin{aligned} &\partial_t Q_{pl} \int_T \phi_l \phi_k \mathrm{d}x - A_{pq} Q_{pl} \int_T \phi_l \partial_x \phi_k \mathrm{d}x \\ &+ \int_{\partial T} F_{pk}(Q_{pl}, Q^i_{pl}) \mathrm{d}s \\ &= E_{pq} Q_{pl} \int_T \phi_l \phi_k \mathrm{d}x \end{aligned}$$