Large Scale Simulations for Applications in Porous Media using the HPC-Software-Framework UG4

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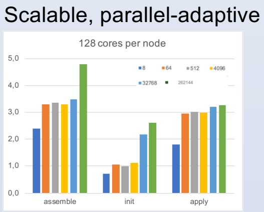
Summary

Simulating subsurface processes involves multiple layers of complexity. These challenges arise from several factors: (1) **Geometric considerations**, including anisotropies and heterogeneities in the porous medium, fractures, thin layers, and moving phreatic surfaces. (2) **Governing equations**, which typically form a transient system of partial differential equations (PDEs) with nonlinear interactions and couplings between physical variables. (3) **Interdependence of geometry and equations**, where the description of the subsurface structure is intrinsically linked to the mathematical formulations. Developing efficient solvers for these problems is nontrivial, requiring careful selection of spatio-temporal discretization methods and linear solvers that can be integrated into high-performance computing (HPC) frameworks.This study presents a unified solver framework that combines scalable multigrid solvers [1,2] in time and space with a linearly implicit extrapolation scheme [3,4]. We demonstrate the effectiveness of this approach across various applications, focusing on flow and transport problems. We assess the robustness of our numerical methods, develop appropriate error estimators, and provide scalability results in an HPC environment.

Classic Numerical Methods

- The software toolbox UG4 [1] provides methods for solving coupled systems of PDEs; Modular organization with tight coupling between FE/FV-discretization and solvers;
- Written in C++ with interface for LUA, Python & Jupyter-Notebooks;
- Scalable, parallel-adaptive multilevel solvers are at its core:



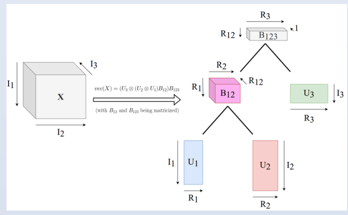
		Uniform	Adaptive	Overhead	Saving
Statistics	# cores	32768	512	—	64
	# nodes	512	8	—	64
	# unknowns	9,104,251,009	187,121,216	—	48.65
	unknowns per core	277,839.7	365,471.1	1.32	—
Times [s]	Assemble	2.85	12.27	4.31	—
	InitPrecond	5.66	9,42	1.66	—
	ApplyPrecond	13.98	17.64	1.26	—
	Integrate	5.43	6.66	1.23	—
	InitBase	3.69	3,65	0.99	—
	ApplyBase	0.17	0.18	1.06	—
	Refine	18.15	29.02	1.60	—
	Distribute	41.84	132.42	3.16	—
	Total (sum)	91.77	211.26	2.30	

Figure 1: Left: Weak scaling of the multigrid solver (Poisson's equation, 3D). Center/right: Impact of adaptivity (skin jumping coefficient problem, 3D). Results on HAWK, HLRS Stuttgart.

- LIMEX-multigrid scheme [3] allows problem-dependent treatment of non-linearities; → increases efficiency and robustness using reduced Jacobian;
- Multigrid Reduction in Time (MGRIT) [4] is an iterative method for solving transient problems; → additional strong scaling due to parallelism in the time domain;
- Monolithic coupling [5] is the default approach for systems of PDEs; → appropriate smoothers must be designed / selected;
- Weak form coupling are strategies can be used, e.g. , for processes w/ timescale disparities → select only after analysis of the rate-limiting processes.

Low rank Approximation for High-dimensional Data

- Hierarchical Tucker Format (HTF) [6] provides compact representation of high-dimensional tensors (multi-dimensional arrays);
- Hierarchically organized data allows efficient arithmetic operations (linear complexity w.r.t. dimension under low-rank assumption)
- Rank-Adaptive-Euler-Scheme [7]: Arithmetics in low-rank tensor format + truncation;
- Benchmark application to diffusion-reaction system from epidemiology yields faster computations, smaller memory footprint and h-dependence;

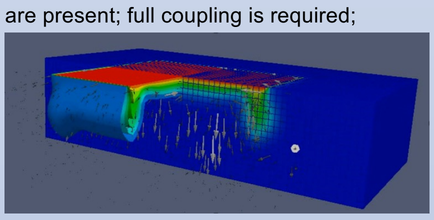


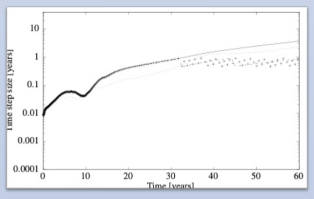
Scheme	Computation speed (#iterations/second)		Memory footprint (in MB)	
Mesh size h	1/128	1/256	1/128	1/256
Classic Forward-Euler	13.87 ± 0.03	3.18 ± 0.02	5450	21630
Rank-Adaptive-Euler	19.03 ± 0.09	13.72 ± 0.14	22	33

- Adaptive cross approximation can be used to compute single quantities of interest, e.g. for UQ; integration into multilevel solvers is ongoing.

Density Driven Flow

- Density effects play an important role, when large gradients in concentration or temperature are present; full coupling is required;





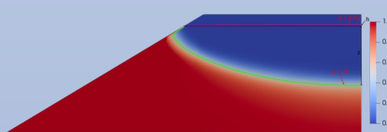
Method	Time steps				Linear solver		Timing	
	q=2	q=3	q=4	reject	success	fail	CPU [s]	Effort
IMPEX	461	—	—	37	3075	36	21228.19	1
$\text{LIMEX}_2^{\text{full}}$	455	—	—	130	1371	129	13564.55	0.64
$\text{LIMEX}_3^{\text{full}}$	75	90	—	131	768	131	7984.37	0.38
$\text{LIMEX}_4^{\text{full}}$	81	7	40	136	708	134	7510.61	0.35
$\text{LIMEX}_2^{\text{reduced}}$	578	—	—	1	1742	0	14375.54	0.68
$\text{LIMEX}_3^{\text{reduced}}$	3	159	—	0	968	0	7464.05	0.35
$\text{LIMEX}_4^{\text{reduced}}$	35	2	63	4	785	0	6115.75	0.29

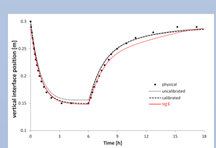
Figure 2: Left: Illustration of density driven flow process (top). Primary unknowns are the fluid pressure p, and salt mass fraction w. Density and viscosity depends on w, resulting in a highly non-linear system.

Right: Solver friendly LIMEX-discretisation with reduced Jacobian yields improved time-stepping and accelerates run times .

- Key ingredients for LIMEX: Fixed velocity approximation for reduced Jacobian; weighted L2- and H1-semi norm for measuring error w.r.t. concentration and pressure.
- A saturation-dependent generalization of the density-driven flow problem extends the method extends to unsaturated media; as for the Richards-Eqn. Additional nonlinearities introduced by water retention curves in the Van Genuchten-model.

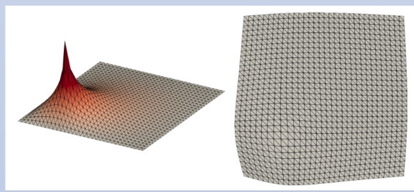
Figure 3.: Left: Development of a fresh water lens under an island. Depicted are phreatic surface (red) and fresh water surface (green). Right: Validation of the transient process with experimental data from (Stoeckl et al., 2012).





Poroelastic Soil Deformation

- Application for the fully coupled, quasi-static Biot equation for Barry-Mercer-benchmark (2D); Discretization with Taylor-Hood- elements (P2-P1) in space, backward Euler in time; (resulting in 9'684'660'224 = 2'364'419 x 4'096 degrees of freedom)



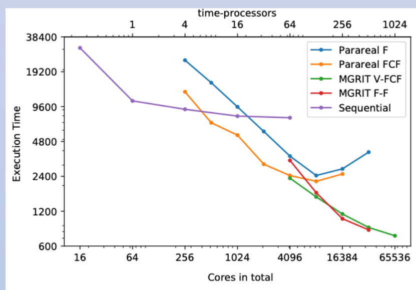
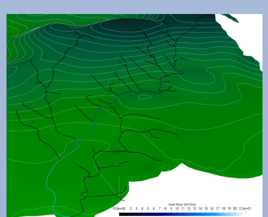


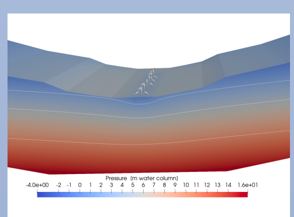
Figure 5: Barry-Mercer benchmark features an oscillating point source triggering a deformation (left). Strong scaling of MGRIT (right).

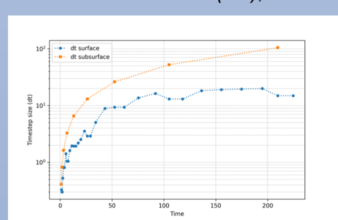
- Multigrid solver with a fixed stress smoother is robust w.r.t size of mesh and time step; yet strong scaling stalls, when the coarse grid solver becomes the bottleneck;
- MGRIT provides additional acceleration:
  Backward Euler: 10,800 seconds on 64 cores (strong scaling limit);
  Parareal (two-level): 2,200 seconds / 4.94 rel. speedup on 8'192 cores;
  MGRIT: 740 seconds / 14.62 rel. speedup on 65'536 cores.

Surface and Subsurface flow

- Weak (iterative) coupling can be used, e.g. for coupling surface and subsurface flow using *St.-Venant-eqn. (1D), shallow-water-eqn. (2D) on surface; unsaturated flow in soil (3D);*



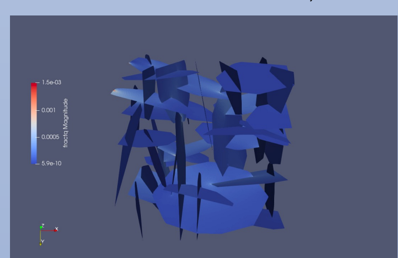




- Separate adaptive LIMEX time integration schemes for surface- and subsurface;
- Exchange fluxes are handled via boundary conditions on the subsurface domain and source terms in the surface equations; iterative boundary condition switching overcomes timescale disparities imposed by different flow velocities.

Transport in Fractured Rocks

- Transport in fracture networks and the surrounding rock matrix require a fully coupled approach; primary unknows: pressure p and concentration c;
- Semi-discrete (reduced dimensional) treatment of fractures allows for conservation of mass and discontinuities across fracture;



Grid level	Degrees of freedom Total	Rock	Fractures	MPI processes	Steps per min
0	152,964	103,233	41,766	—	—
1	844,479	652,245	165,747	—	—
2	5,277,660	40,29,300	1,153,050	128	0.167
3	36,388,506	29,943,414	6,085,020	1024	0.150
4	267,939,174	238,762,698	27,778,416	8192	0.158

Figure 3.: Left: Visualiization of transport in a network of 45 fractures. Rock matrix excluded for the sake of visual convenience Top: Result of weak scaling.

- Time-stepping in LIMEX-multigrid is h-dependent (data not shown); Problem can be solved with robust weak scaling.

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