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Parallelization schemes in OpenGeoSys and applications to density driven and reactive flows in geosystems.

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OpenGeoSys (OGS) is an open-source multi-platform modelling package for solving individual or coupled thermo-hydro-mechanical-chemical/biological (THM/CB) processes in porous and fractured media. OGS is used in various geoscientific applications such as groundwater management, geo-energy resources, geological storage and energy waste management. Currently the new version OGS-6 is under development (www.opengeosys.org, docs.opengeosys.org).

Currently, the strongly coupled PDEs of large-scale processes are solved using MPI distributed memory parallelization. In this presentation, we propose a combined shared and distributed memory approach using MPI and OpenMP in order to benefit from new generation of architectures, like Intel's Xeon Phi Knights Landing.

We could demonstrate that for specific applications the combination of OpenMP with MPI has advantages, especially if the OpenMP tasks are highly parallelisable. This has been shown, *e*.g. in the coupling of IPHREEQC and OGS where the chemical solver was parallelized with OpenMP and the PDEs domain was partitioned.

The simulations were conducted on different HPC facilities. These benchmarks show that the proposed combined approach is advantageous over the classical MPI parallelization in terms of reduced computational time, especially if the OpenMP tasks are highly parallelizable. We believe that large-scale simulations of coupled processes, *e*.g. THM-C, will strongly benefit from the proposed scheme.