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Efficient development of memory bounded geo-applications to scale on modern supercomputers

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Numerical modeling is an actual key tool in the area of geosciences. The current challenge is to solve problems that are multi-physics and for which the length scale and the place of occurrence might not be known in advance. Also, the spatial extend of the investigated domain might strongly vary in size, ranging from millimeters for reactive transport to kilometers for glacier erosion dynamics. An efficient way to proceed is to develop simple but robust algorithms that perform well and scale on modern supercomputers and permit therefore very high-resolution simulations.

We propose an efficient approach to solve memory bounded real-world applications on modern supercomputers architectures. We optimize the software to run on our newly acquired state-of-the-art GPU cluster "octopus". Our approach shows promising preliminary results on important geodynamical and geomechanical problematics: we have developed a Stokes solver for glacier flow and a poromechanical solver including complex rheologies for nonlinear waves in stressed rocks porous rocks.

We solve the system of partial differential equations on a regular Cartesian grid and use an iterative finite difference scheme with preconditioning of the residuals. The MPI communication happens only locally (point-to-point); this method is known to scale linearly by construction. The "octopus" GPU cluster, which we use for the computations, has been designed to achieve maximal data transfer throughput at minimal hardware cost. It is composed of twenty compute nodes, each hosting four Nvidia Titan X GPU accelerators. These high-density nodes are interconnected with a parallel (dual-rail) FDR InfiniBand network.

Our efforts show promising preliminary results for the different physics investigated. The glacier flow solver achieves good accuracy in the relevant benchmarks and the coupled poromechanical solver permits to explain previously unresolvable focused fluid flow as a natural outcome of the porosity setup. In both cases, near peak memory bandwidth transfer is achieved. Our approach allows us to get the best out of the current hardware.