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In Situ and In Transit Computing for Large Scale Geoscientific Simulation

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In situ and in transit computing is an effective way to place postprocessing and preprocessing tasks for large scale simulations on the high performance computing platform. The resulting proximity between the execution of preprocessing, simulation and postprocessing permits to lower I/O by bypassing slow and energy inefficient persistent storages. This permits to scale workflows consisting of heterogeneous components such as simulation, data analysis and visualization, to modern massively parallel high performance platforms. Reordering the workflow components gives a manifold of new advanced data processing possibilities for research. Thus in situ and in transit computing are vital for advances in the domain of geoscientific simulation which relies on the increasing amount of sensor and simulation data available.

In this talk, different in situ and in transit workflows, especially those that are useful in the field of geoscientific simulation, are discussed. Furthermore our experiences augmenting ParFlow-CLM, a physically based, state-of-the-art, fully coupled water transfer model for the critical zone, with FlowVR, an in situ framework with a strict component paradigm, are presented.
This allows shadowed in situ file writing, in situ online steering and in situ visualization.

In situ frameworks further can be coupled to data assimilation tools.
In the on going EoCoE-II we propose to embed data assimilation codes into an in transit computing environment. This is expected to enable ensemble based data assimilation on continental scale hydrological simulations with multiple thousands of ensemble members.