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Enhancing parallel execution of the coupled PCR-GLOBWB-MODFLOW at global extent and high resolution simulations

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PCR-GLOBWB (PCRaster Global Water Balance, https://github.com/UU-Hydro/PCR-GLOBWB_model) is a large-scale hydrological model developed at the Department of Physical Geography, Utrecht University, the Netherlands. The latest version of the model can simulate terrestrial hydrological and water resource storages and fluxes at the global extent with 5 arc-min (less than 10 km) spatial resolution and daily temporal resolution.

One of the recent features in the PCR-GLOBWB model development is the inclusion of a global 2-layer MODFLOW model simulating groundwater lateral flow and allowing assessment of groundwater head changes at the global extent, including regions with declining groundwater head problems. Unfortunately, the current coupled PCR-GLOBWB-MODFLOW requires significant run times mainly attributed to the current inefficient serial coupling scheme. Currently, to reduce computational time for a global extent simulation, the groundwater simulation is compromised by using a monthly MODFLOW stress period in which daily simulation values (e.g. surface water levels, groundwater recharge and abstraction) of PCR-GLOBWB are aggregated. Consequently, prediction ability and modelling accuracy is limited, e.g. water balance errors are induced as an explicit scheme is used to exchange fluxes between daily PCR-GLOBWB and monthly MODFLOW simulation.

In this work, we aim to improve the coupled PCR-GLOBWB-MODFLOW model by setting-up a favorable river-basin partitioning that reduces I/O communication and optimizes load balance between PCR-GLOBWB and MODFLOW. We also aim to replace the MODFLOW-2000 in the current coupled model with the newest parallel MODFLOW 6, that is being developed together with the USGS and uses Message Passing Interface (MPI).. The latest scaling test carried out on the Cartesius Dutch National supercomputer shows that the usage of parallel MODFLOW 6 can result in significant MODFLOW calculation speedups (up to a factor of 45). The encouraging result of this work opens a possibility for running the model with higher temporal resolution, i.e. daily simulation of MODFLOW. Moreover, as MODFLOW 6 supports both structured and unstructured grids, this development includes an opportunity to have a next generation of PCR-GLOBWB-MODFLOW model that has flexibility in grid design for its groundwater flow simulation (e.g. grid design can be used to focus along rivers and around wells, to discretize individual layers to better represent hydrogeological units).