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Advanced parallel computing for the coupled PCR-GLOBWB-MODFLOW model

Jarno Verkaik (1), Oliver Schmitz (2), and Edwin Sutanudjaja (2)

(1) Deltares, Delft, The Netherlands (jarno.verkaik@deltares.nl), (2) Department of Physical Geography, Utrecht University, The Netherlands

PCR-GLOBWB (https://github.com/UU-Hydro/PCR-GLOBWB_model) is a large-scale hydrological model intended for global to regional studies and developed at the Department of Physical Geography, Utrecht University (Netherlands). The latest version of the model can simulate terrestrial hydrological and water resource fluxes and storages with a typical spatial resolution of 5 arc-minutes (less than 10 km) at the global extent. One of the recent features in the model development is the inclusion of a global 2-layer MODFLOW model simulating groundwater lateral flow. This advanced feature enables us to simulate and assess the groundwater head dynamics at the global extent, including at regions with declining groundwater head problems.

Unfortunately, the current coupled PCR-GLOBWB-MODFLOW requires long run times mainly attributed to the current inefficient parallel computing and coupling algorithm. In this work, we aim to improve it by setting-up a favorable river-basin partitioning manner 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 MODFLOW-USG. This will allow us to use the new Parallel Krylov Solver (PKS) that can run with Message Passing Interface (MPI) and can be easily combined with Open Multi-Processing (OpenMP). The latest scaling test carried out on the Cartesius Dutch National supercomputer shows that the usage of MODFLOW-USG and new PKS solver can result in significant MODFLOW calculation speedups (up to 45). The encouraging result of this work opens a possibility for running the model with more detailed setup and at higher resolution. As MODFLOW-USG supports both structured and unstructured grids, this 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).