Parallel Multi-physics Simulations using OpenPALM with Application to Hydro-biogeochemistry Coupling

M. Wlotzka[1] **and V. Heuveline**[2]

Abstract: Multi-physics systems consist of more than one component governed by its own principle for evolution or equilibrium. As an example, we consider an agricultural land use scenario comprising a hydrology model and a biogeochemistry model. Current practices for multi-physics coupling seek to find a balance between performance, numerical accuracy and software reuse. The OpenPALM coupling tool allows to perform parallel multi-physics simulations employing specialized model implementations as well as legacy codes.

We consider surface and subsurface water flow and transport of chemical species in the hydrology model. Microbial and physiochemical processes in the soil and plant growth are considered in the biogeochemical model. Spatial discretization leads to the semi-discretized formulation

$$\partial_t(w,s) = f_{\mathsf{hyd}}(w,s,t) \qquad \text{(hydrology)}\,, \tag{13}$$

$$\partial_t s = f_{\mathsf{bgc}}(w,s,t) \qquad \text{(biogeochemistry)}\,, \tag{14}$$

with soil water content w and chemical species concentration s. To address the coupled problem numerically, we propose the following operator splitting solution scheme:

Algorithm 2 Concurrent operator splitting scheme

Given initial states $w(t_0) = w_0$, $s(t_0) = s_0$.
for n=0,1,...,N **do**
    Solve (13) using $w(t_n) = w_n$, $s(t_n) = s_n$ for one time-step to obtain w_{n+1}, $\hat{s}_{n+1}$.
    Solve (14) using $w \equiv w_n$, $s(t_n) = s_n$ for one time-step to obtain $\tilde{s}_{n+1}$.
    Set $s_{n+1} = \hat{s}_{n+1} + \tilde{s}_{n+1} - s_n$.
end for

This solution scheme is of first order in time for the coupled evolution problem. Since the models can be solved concurrently within each iteration, this operator splitting scheme offers a second level of parallelism, in addition to parallelizing the computations for each individual model.

In our presentation, we demonstrate the use of the OpenPALM coupling tool to implement the proposed solution scheme. We investigate the parallel performance and efficiency of our solution scheme based on numerical experiments on shared memory multi-core architectures and on distributed memory machines. The underlying hydrology and biogeochemistry models are based on the Catchment Modelling Framework and the LandscapeDNDC ecosystem model, respectively.

[1,2] Interdisciplinary Center for Scientific Computing, University of Heidelberg
Speyerer Str. 6, 69115 Heidelberg, Germany
martin.wlotzka@uni-heidelberg.de, vincent.heuveline@uni-heidelberg.de