Contributions from WP1 to applications from WP4
Example applications: ParFlow and SHEMAT-Suite

Rene Halver[3] Wendy Sharples[1,2,3]
Contributing authors: Jose Fonseca[3], Ketan Kulkarni[2], Sebastian Luehrs[2], Damian Kalizan[4]

(1) Centre for High-Performance Scientific Computing in Terrestrial Systems, Geoverbund ABC/J; (2) Jülich Supercomputing Centre (JSC), (2) Forschungszentrum Jülich; (3) Meteorological Institute, Bonn University; (4) Poznan Supercomputing and Networking Center

ParFlow: Description

A parallel 3D variably saturated ground water flow model, ParFlow includes fully-integrated overland flow, the ability to simulate complex topography, geologic heterogeneity and coupled land-surface processes.

ParFlow is MPI parallel and uses a binary and netCDF IO formats.

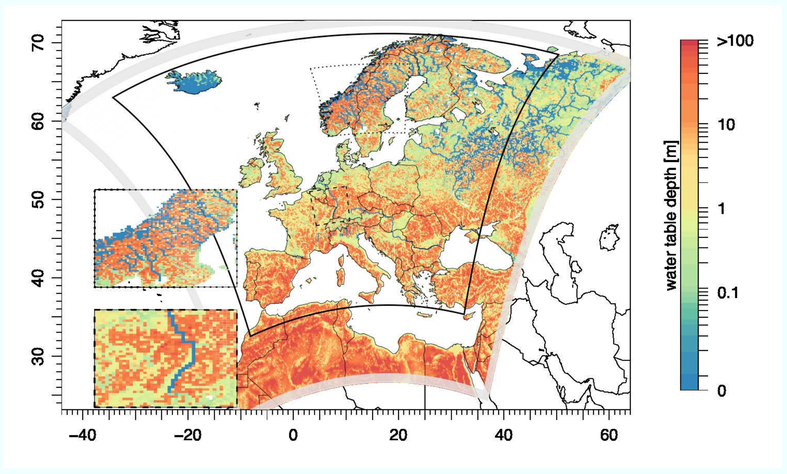
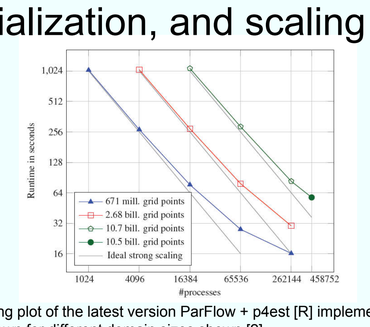


Figure depicting multiscale features of the simulated water table depth across the EuroCordex domain, snapshot taken from 10th August 2003 [1]

WP1 contribution to ParFlow

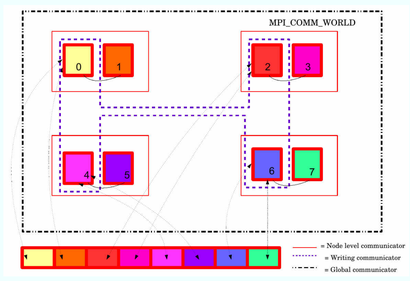
Towards Exascale:

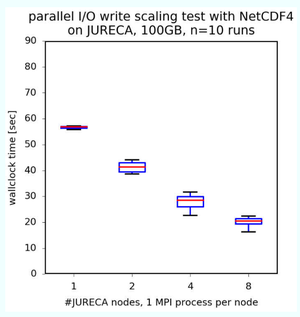
- Integrating ParFlow with p4est to improve memory management, initialization, and scaling



Scaling plot of the latest version ParFlow + p4est [R] implementation. Total runtime is shown for different domain sizes shown [2]

- Rising to the big data challenge by implementing parallel NetCDF4 I/O

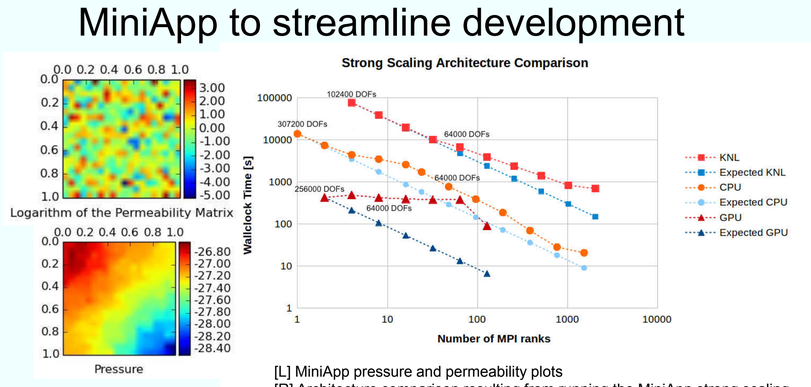




[L] Diagram of the collective output implementation of parallel NetCDF4 I/O
[R] NetCDF4 scaling benchmark (Ketan Kulkarni JSC)

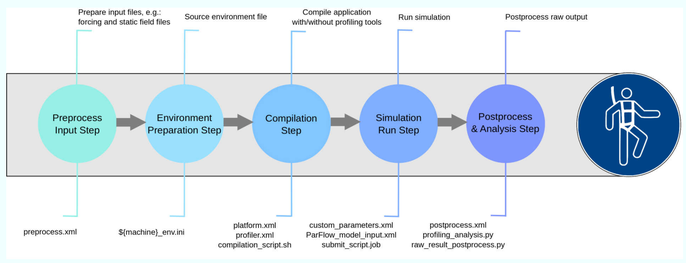
Next generation hardware and software:

- Adapting ParFlow to next generation hardware and software with a MiniApp to streamline development



[L] MiniApp pressure and permeability plots
[R] Architecture comparison resulting from running the MiniApp strong scaling benchmark across CPUs, GPUs and KNLs (Wendy Sharples JSC, Damian Kalizan PSNC)

- Developing a run control framework for porting, profiling, tuning and provenance tracking



Run control framework for the complete modelling chain implemented. Describes each step in the chain (xml files and scripts) [3]

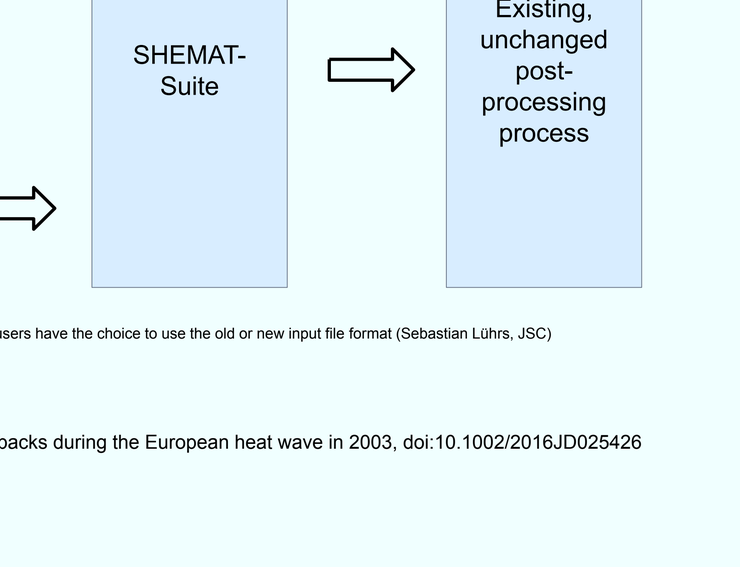
SHEMAT-Suite: Details

- Simulation code for flow, heat and species transport through porous media
- Parallelised with MPI and OpenMP
- Uses custom input format as well as basic HDF5 for sequential I/O
  → bottleneck for large simulations

Permeability distribution of the Sleipner reservoir. [4]

WP1 contribution to SHEMAT-Suite

- Conversion of old input format to enhanced HDF5 input format
- Provided a converter to transform old input file format into new HDF5 format
- Work in progress: conversion of sequential I/O to parallel I/O to allow for better scalability by reducing the per-core memory footprint



Impact of the new input file format on I/O time (Sebastian Lührs, JSC)

Program flow with the inclusion of the WP1 contributions (turquoise); users have the choice to use the old or new input file format (Sebastian Lührs, JSC)

References

[1] Keune, J., F. Gasper, K. Goergen, A. Hense, P. Shrestha, M. Sulis, and S. Kollet (2016), Studying the influence of groundwater representations on land surface-atmosphere feedbacks during the European heat wave in 2003, doi:10.1002/2016JD025426
[2] Burstedde, C., Fonseca, J.A. & Kollet, S. Comput Geosci (2017). https://doi.org/10.1007/s10596-017-9696-2
[3] Sharples, W., Zhukov, I., Geimer, M., Goergen, K., Kollet, S., Luehrs, S., Breuer, T., Naz, B., Kulkarni, K., and Brdar, S (2017). 10.5194/gmd-2017-242, in review.
[4] Büsing, Henrik & Clauser, Christoph. (2017). Efficient Solution Techniques for Multi-Phase Flow in Porous Media. 10.13140/RG.2.2.12988.54405.

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