

# Contributions from WP1 to applications from WP4

## Example applications: ParFlow and SHEMAT-Suite

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### 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.

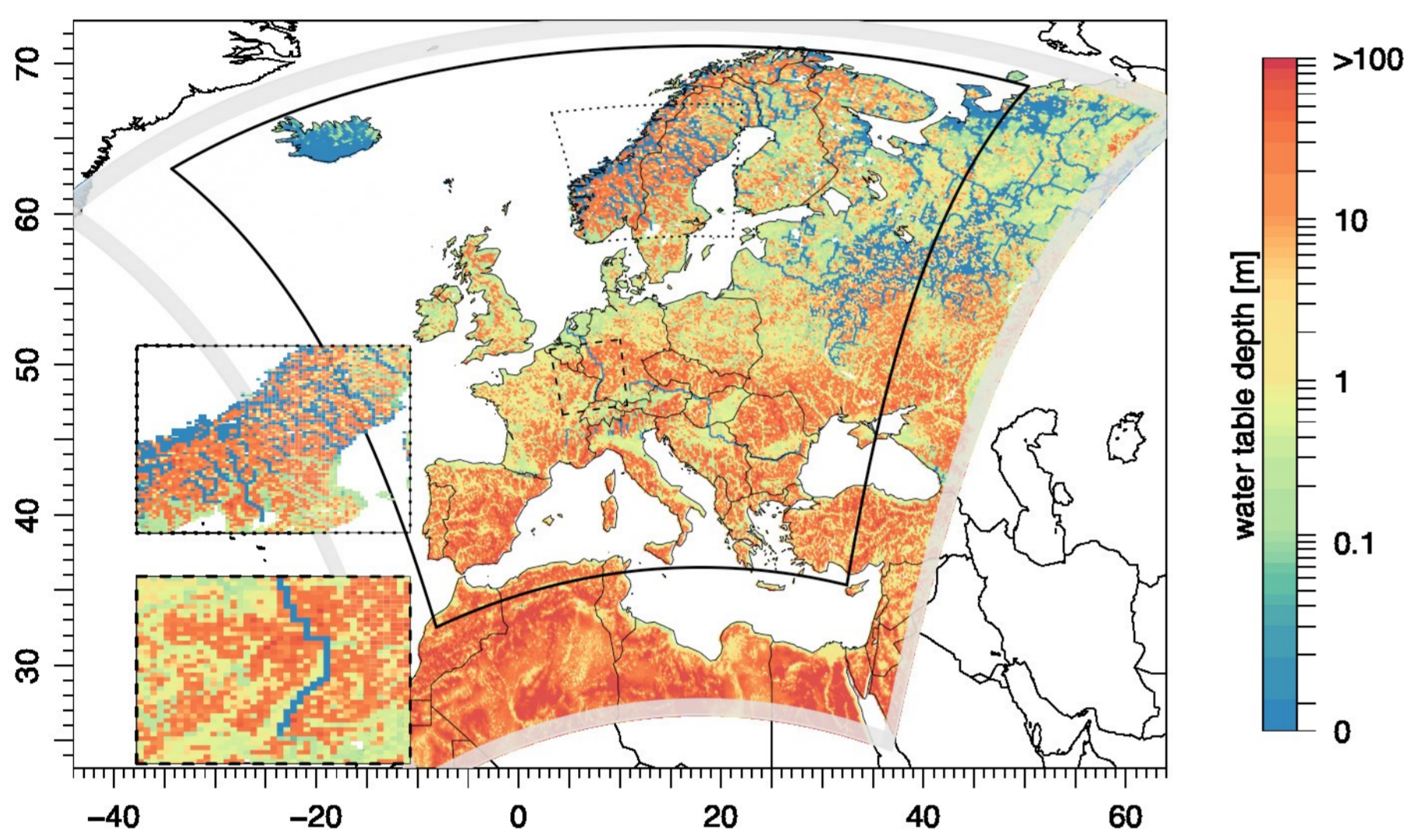
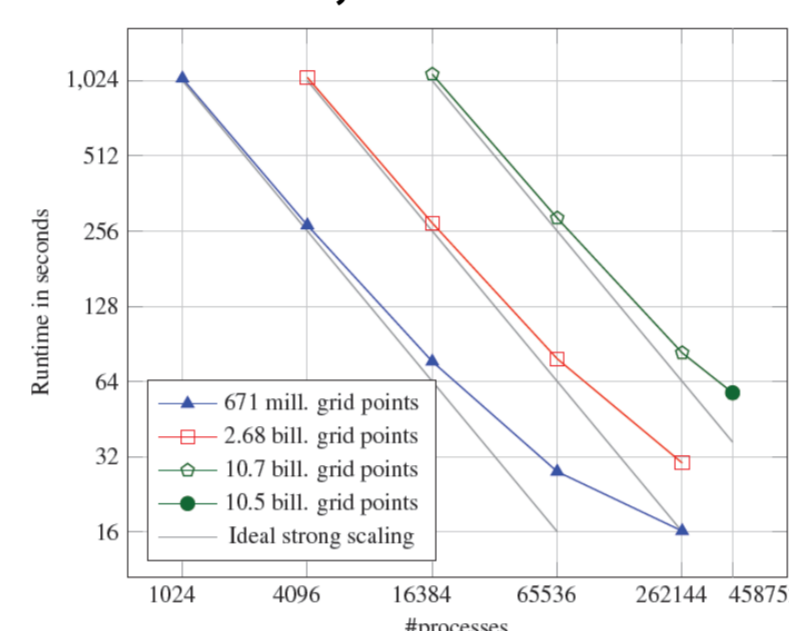


Figure depicting multiscale features of the simulated water table depth across the EuroCordex domain, snapshot taken from 10<sup>th</sup> August 2003 [1]

### WP1 contribution to ParFlow

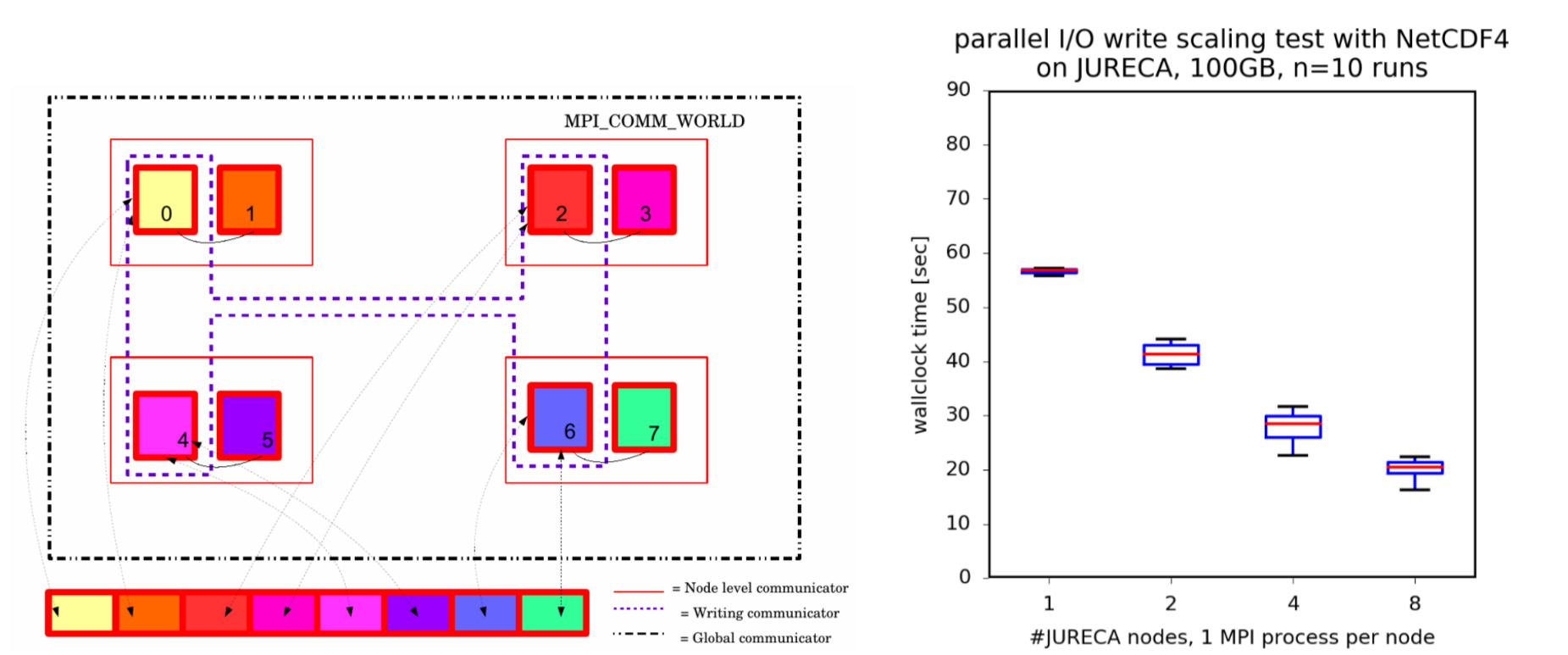
#### Towards Exascale:

- 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]

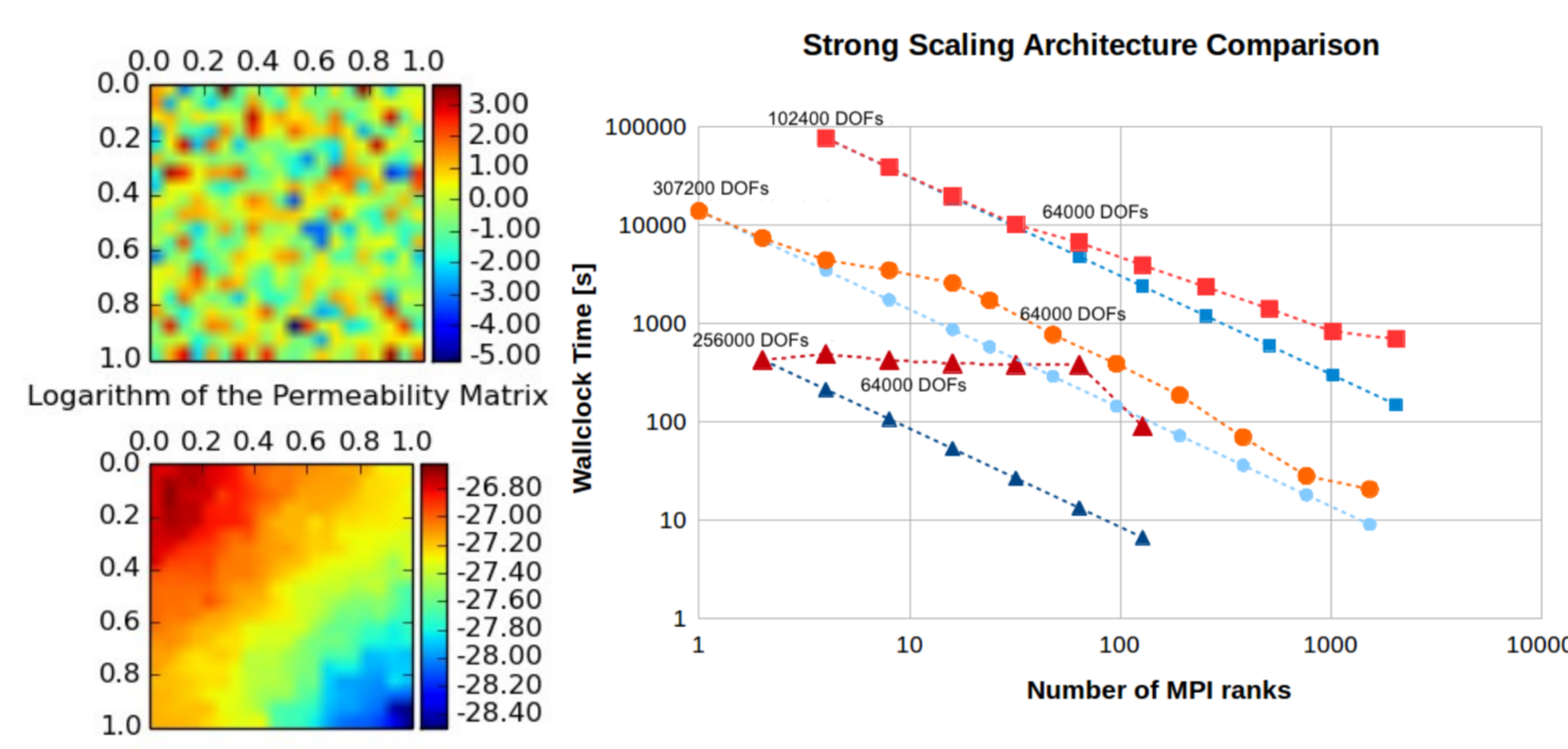
- Rising to the big data challenge by implementing parallel NetCDF4 I/O



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

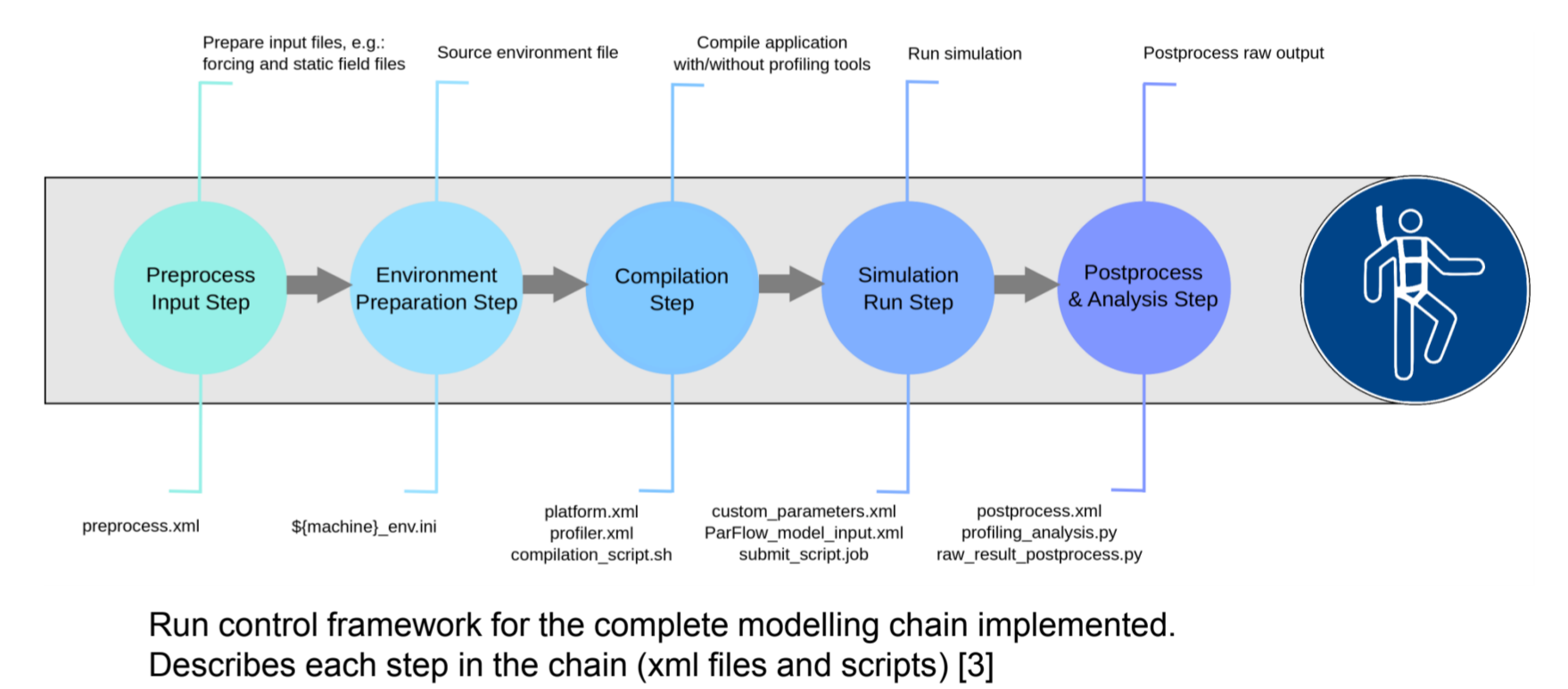
#### Next generation hardware and software:

- 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



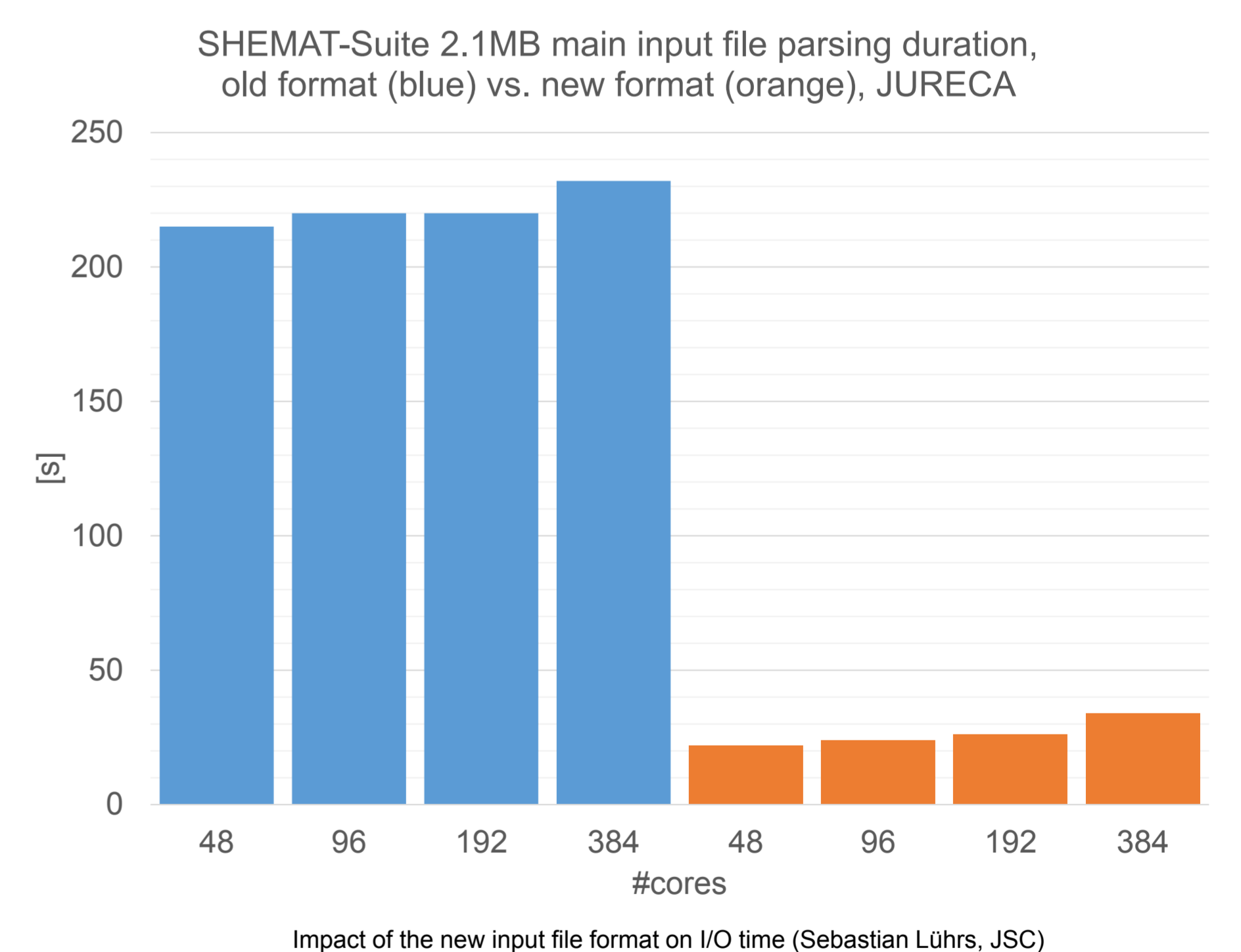
Run control framework for the complete modelling chain implemented. Describes each step in the chain (xml files and scripts) [3]

### SHEMAT-Suite: Details

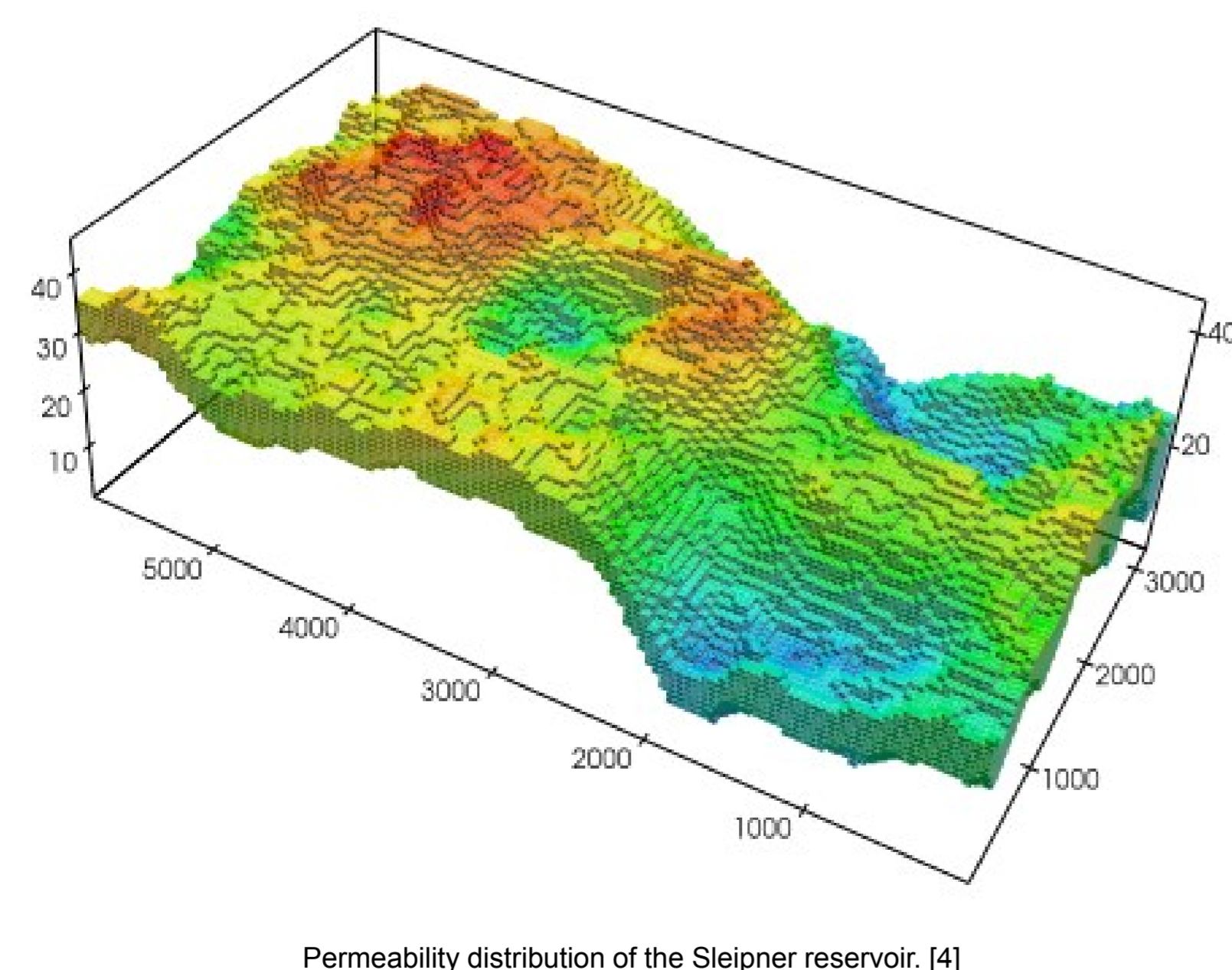
- Simulation code for flow, heat and species transport through porous media
- Parallelised with MPI and OpenMP
- Uses custom input format as well as basic HDF5 for sequential I/O → bottleneck for large simulations

### WP1 contribution to SHEMAT-Suite

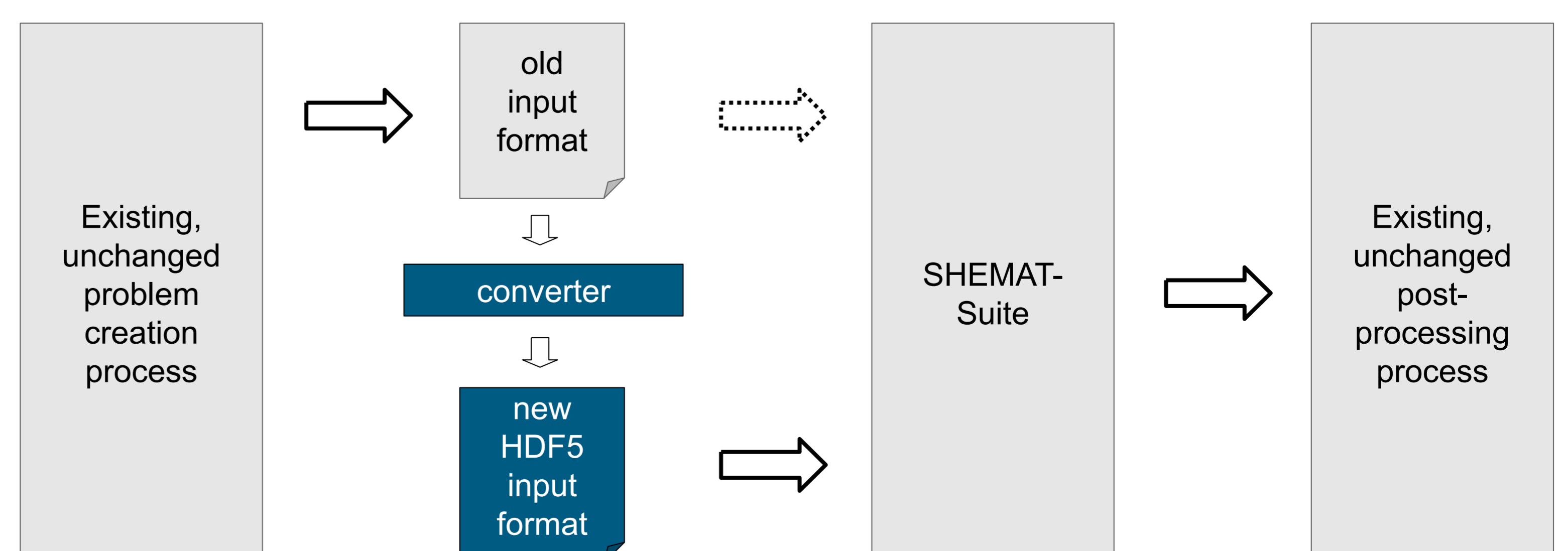
- Conversion of old input format to enhanced HDF5 input format
- Provided a converter to transform old input file format into new HDF5 format
- Work in progress: conversion of sequential I/O to parallel I/O to allow for better scalability by reducing the per-core memory footprint



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



Permeability distribution of the Sleipner reservoir. [4]



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