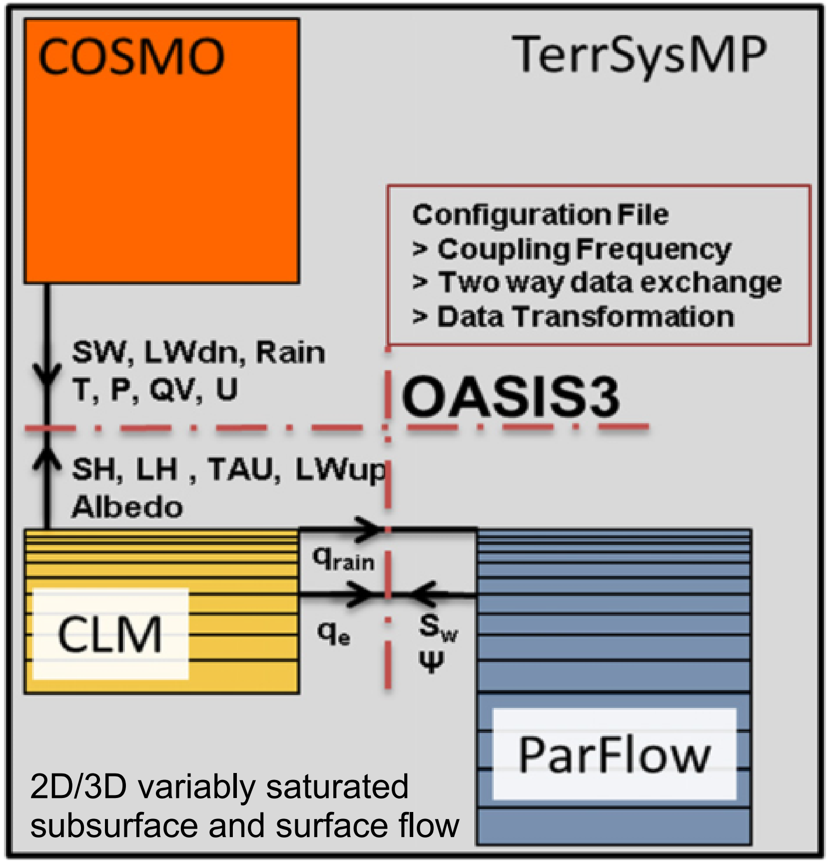
Fully coupled terrestrial water cycle simulations with TerrSysMP: Technical aspects and applications

April 7, 2016 | Ketan Kulkarni[1,4], Klaus Goergen[1,2,4], Fabian Gasper[3,4], Jessica Keune[2,4], Wolfgang Kurtz[3], Lukas Poorthuis[1,4], Bernd Schalge[2], Wendy Sharples[1,4], Prabhakar Shrestha[2], Mauro Sulis[2], Markus Übel[2], Harrie-Jan Hendricks-Franssen[3,4], Clemens Simmer[2,4], Stefan Kollet[3,4]

[1] SimLab TerrSys, Jülich Supercomputing Centre, Research Centre Jülich
[2] Meteorological Institute, University of Bonn
[3] Agrosphere (IBG-3), Research Centre Jülich
[4] Centre for High Performance Scientific Computing in Terrestrial Systems (Geoverbund ABC/J)

TerrSysMP structure
Three component models, some design features

Three component models
OASIS external, parallel coupler
sequentially passes states and fluxes



Shrestha et al. (2014, Mon Weather Rev)

Coupling interface: OASIS3 / OASIS3-MCT (driver)

- Uses MPMD execution model
- Suitable for independently developed codes
- Implementation is less code-intrusive
- Component Models can have different spatio-temporal resolution
- Sub-cycling, temporal averaging, grid interpolation possible
- Downscaling option also implemented
- MPI-1 and MPI-2 possible
- OASIS3 creates MPI_COMM_WORLD
- Various configuration options (component models standalone and combinations)
- Modular coupling design

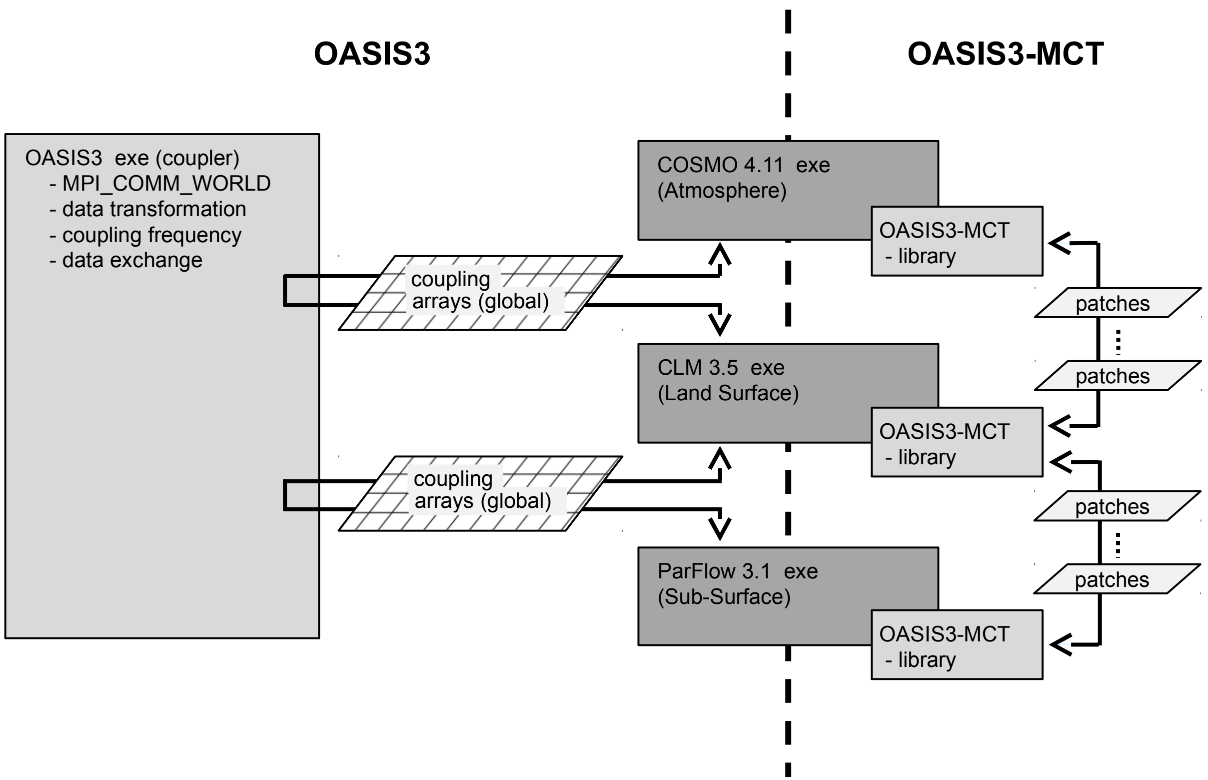
Production use on various HPC architectures

Further code developments (DA, CO2)

Continuous HPC optimisations

Coupling scheme

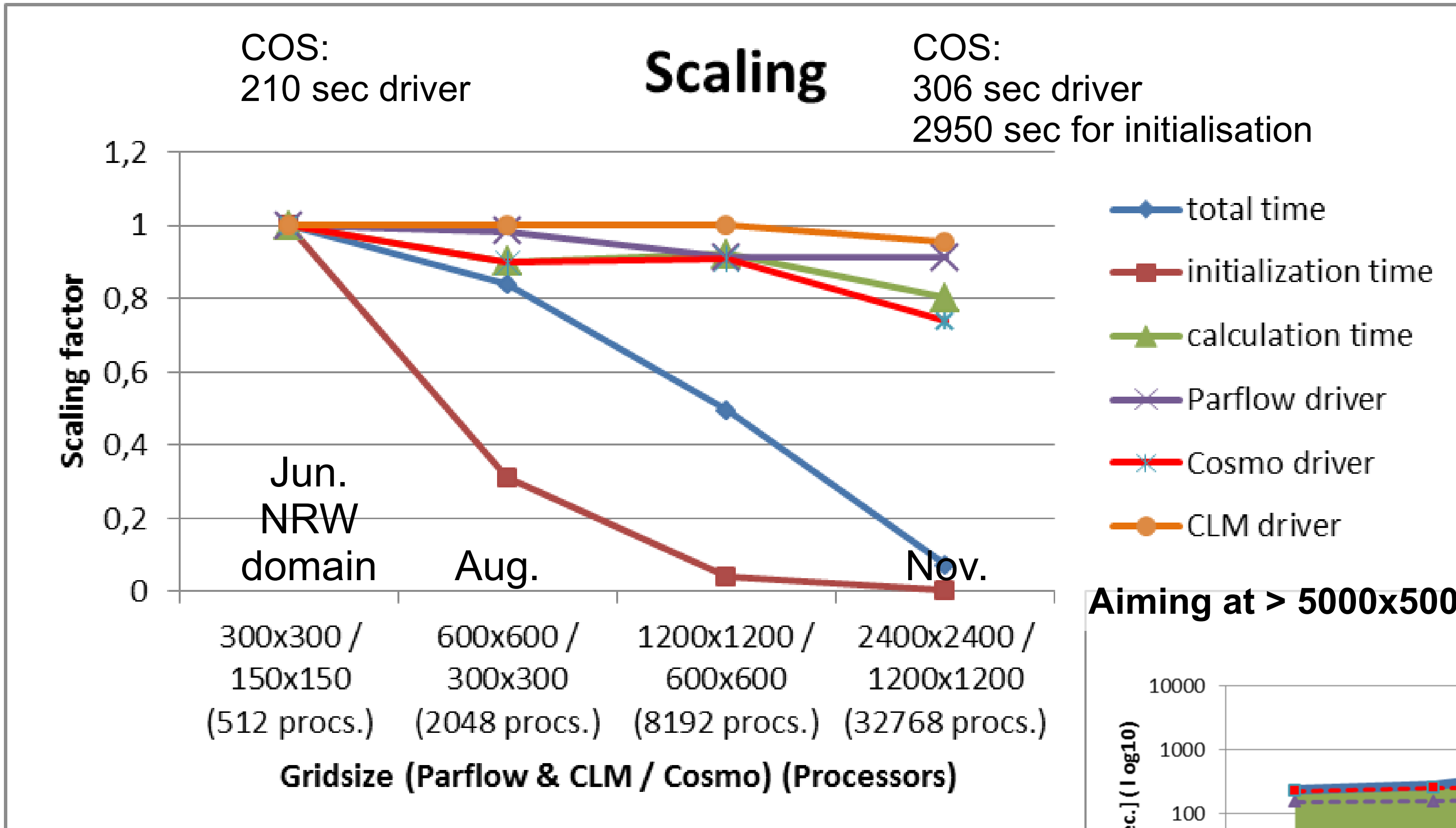
- All combinations possible:
  - COSMO standalone
  - CLM standalone
  - Parflow standalone
  - COSMO/CLM
  - CLM/ParFlow
  - Fully coupled



F. Gasper et al. (2014, GMD)

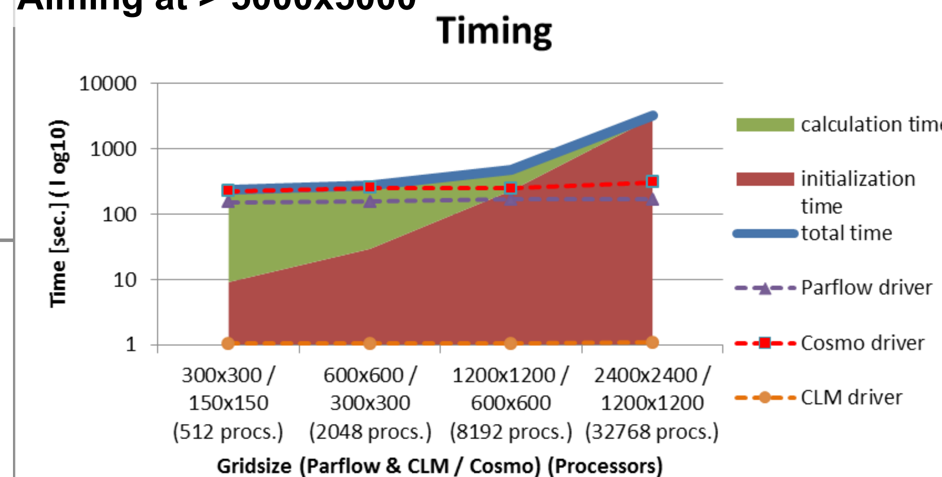
JÜLICH FORSCHUNGSZENTRUM

TerrSysMP HPC optimisations, e.g. IBM BG/Q Good scaling: large domains, high res., long runtimes



- Idealized test case
- 3 h simulation time
- 1 km COS
  0.5 km CLM, PFL
- Weak scaling
- Optimally balanced
- Increase of domain size by factor of 4 (64x overall wrt our unit size)
- No I/O for largest runs

Aiming at > 5000x5000



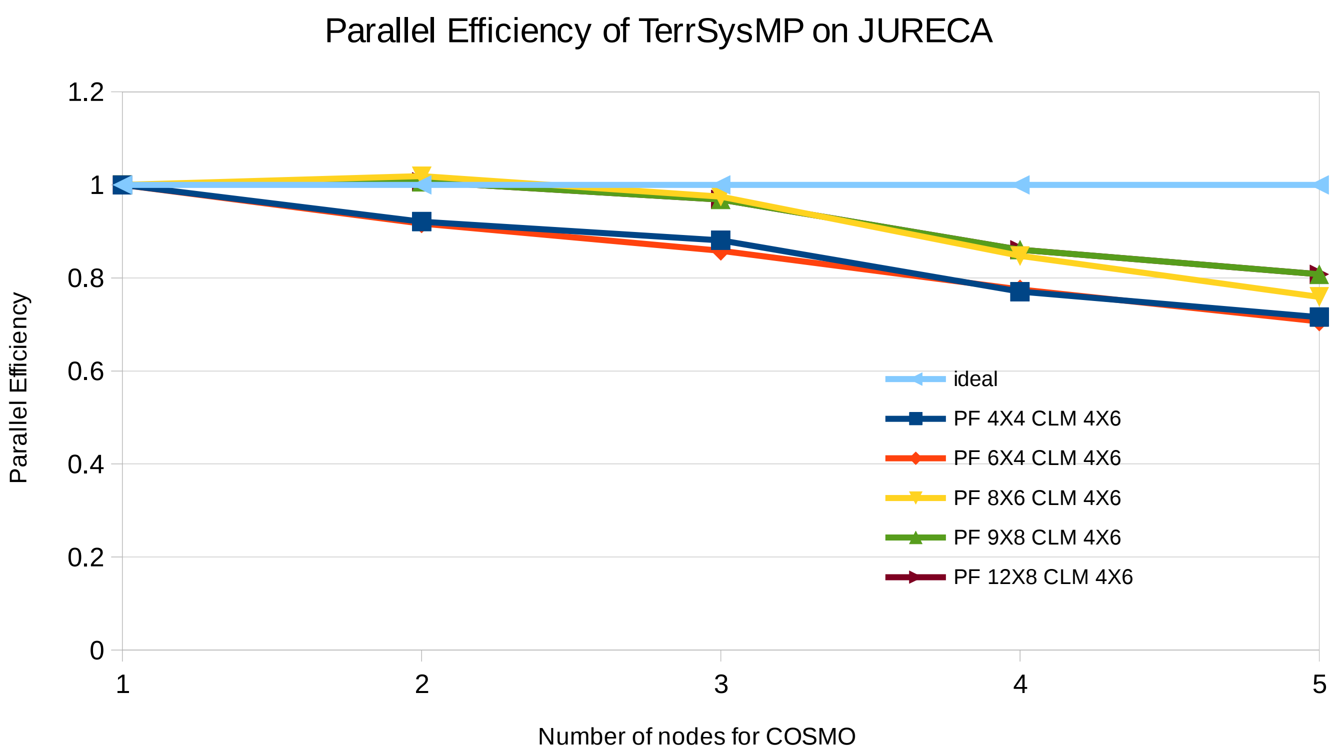
- OASIS3-MCT coupler
- COS 22x16, CLM 80, PFL 8x8 (basic resource assignment for 300x300/150x150 from Scalasca)
- SMT1, ranks per node 16
- 900 sec coupling frequency

F. Gasper et al. (2014, GMD)

Encouraging weak scaling behaviour, 1 month simulation time = 1 day wallclock

JÜLICH FORSCHUNGSZENTRUM

Strong Scaling behaviour on JURECA

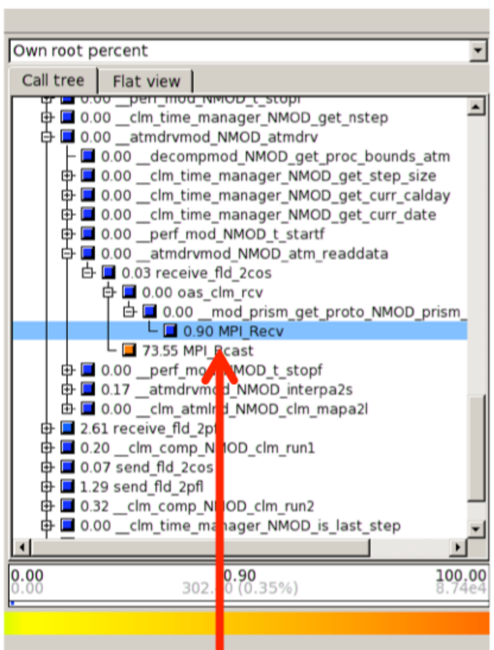


- NRW Standard test case
- 150X150 COSMO
- 300X300 CLM and ParFLOW

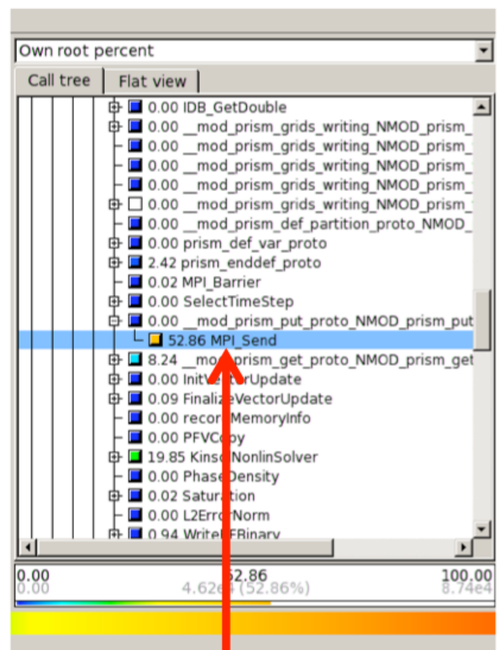
- JURECA = General purpose Linux cluster with commodity hardware
- Two Intel Xeon E5-2680 v3 Haswell CPUs per node (2 X 12 cores @2.5 Ghz, AVX2.0)
- 128 GB DDR4 RAM per node
- Mellanox EDR InfiniBand with non-blocking fat tree topology

"Load balancing" for MPMD using Scalasca/Score-P
How many processes per component model?

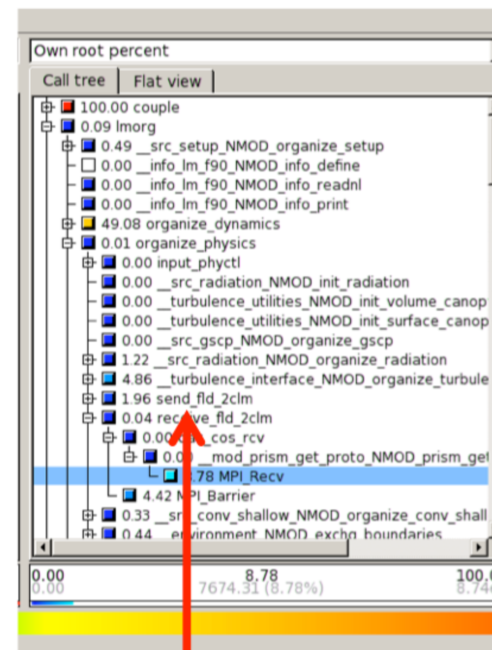
- Let the Model run for a representative number of timesteps
- Interrogating the profile leads to in-depth knowledge of waits/code bottlenecks
- With this method we were able to reduce the runtime by 16% compared to a balancing based on "hand written" timings



CLM waits 73% of the time for Cosmo



Parflow waits 53% of the time for CLM (and CLM waits for Cosmo)

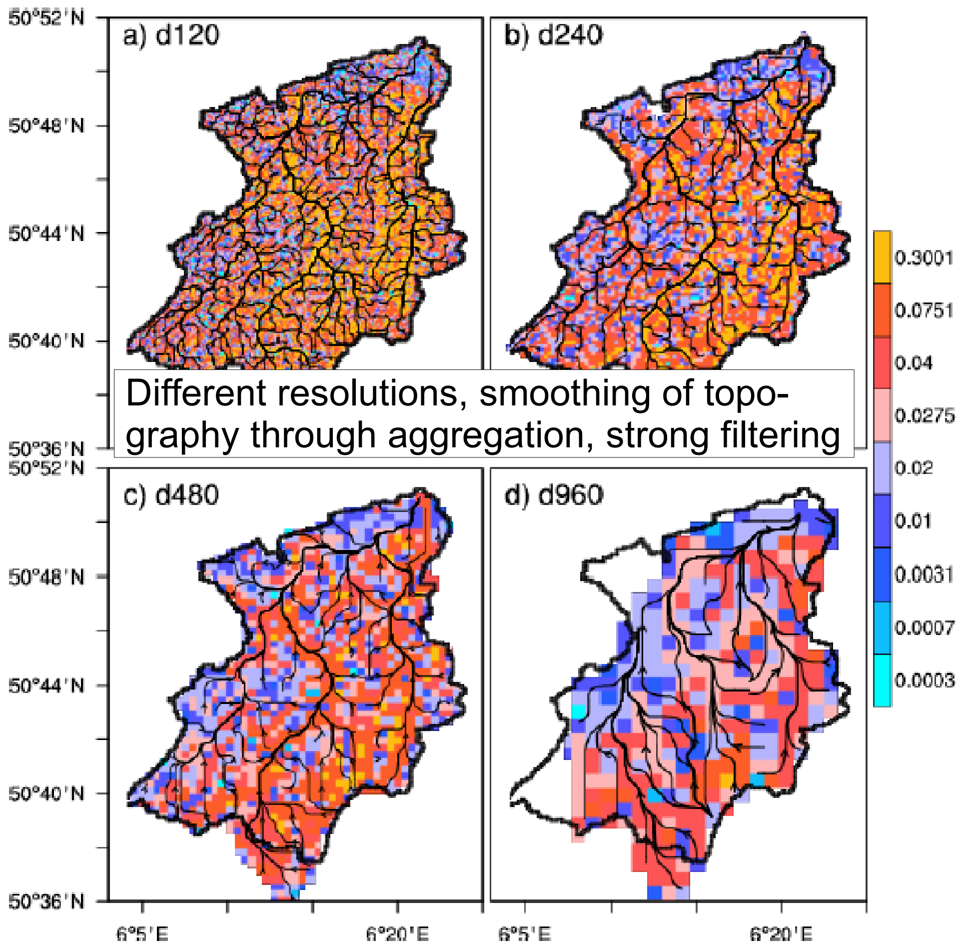


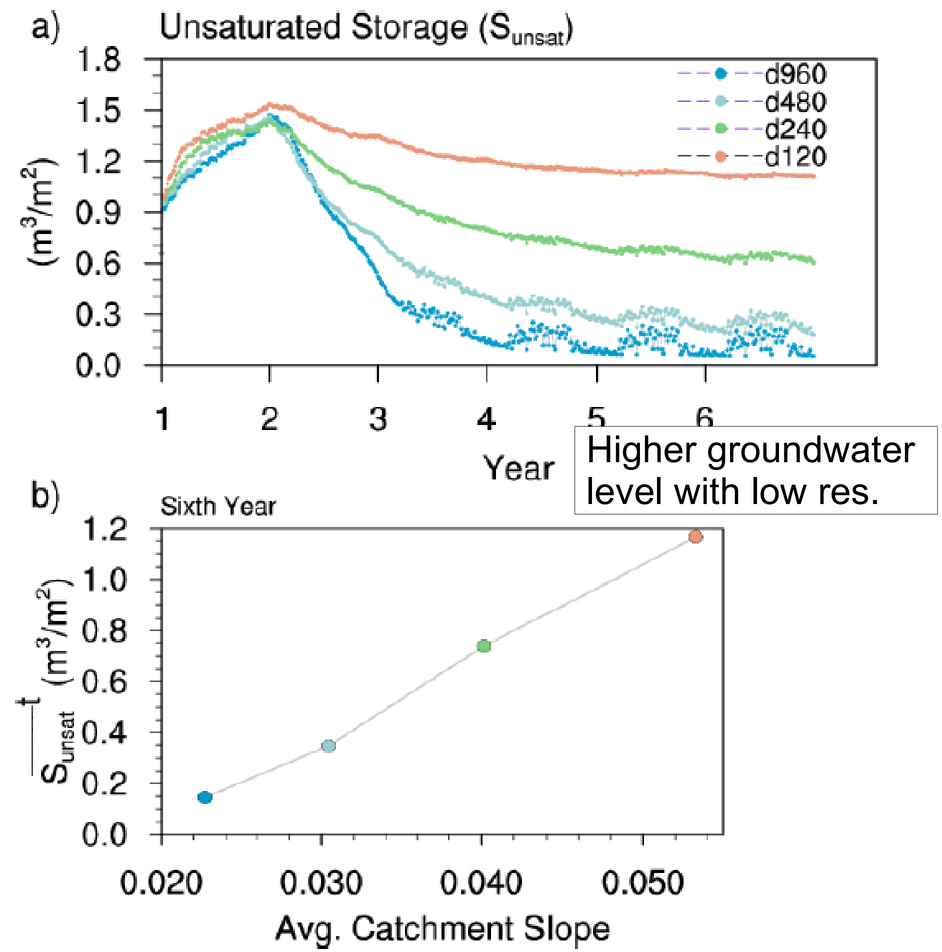
Cosmo does not have to wait (slowest)

Properties and impacts of the fully coupled model: Sensitivity studies on water cycle processes in the terrestrial system (focus PBL interactions, L-A coupling)

TerrSysMP validation and sensitivity
Resolution effects on surface energy fluxes

- ParFlow+CLM; small-scale surface heterogeneities and properties significantly affect surface run-off and infiltration and subsurface redistribution leading to different coupling regimes





325 km2, Wehebach, Rur catchment, uniform subsurface
COSMO-DE periodic upper boundary forcing, dt=1hr, 2.8km

P. Shrestha et al. (2015, HESS)

TerrSysMP sensitivity and improvements
Impact on fluxes through heterogeneity and resolution

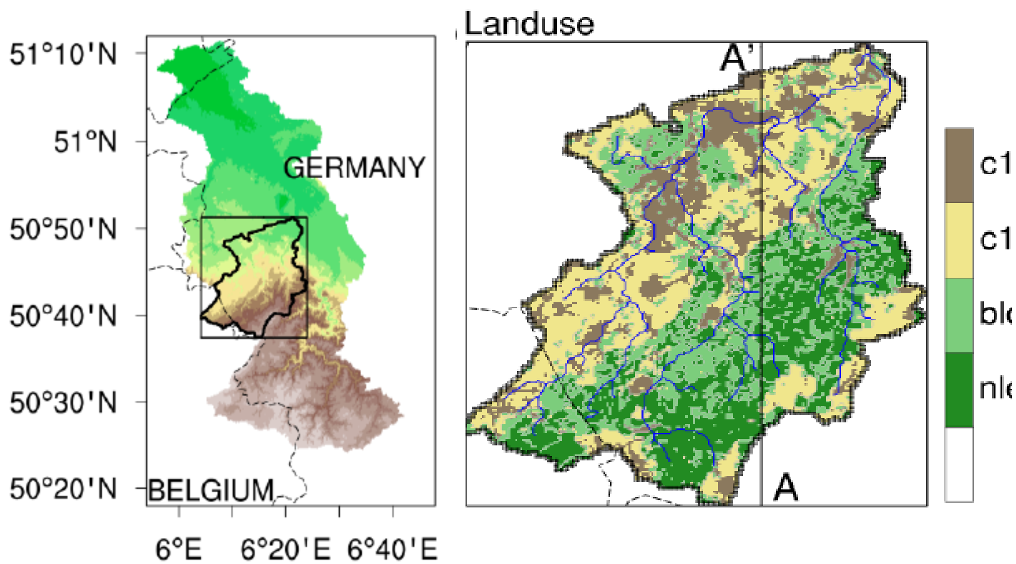
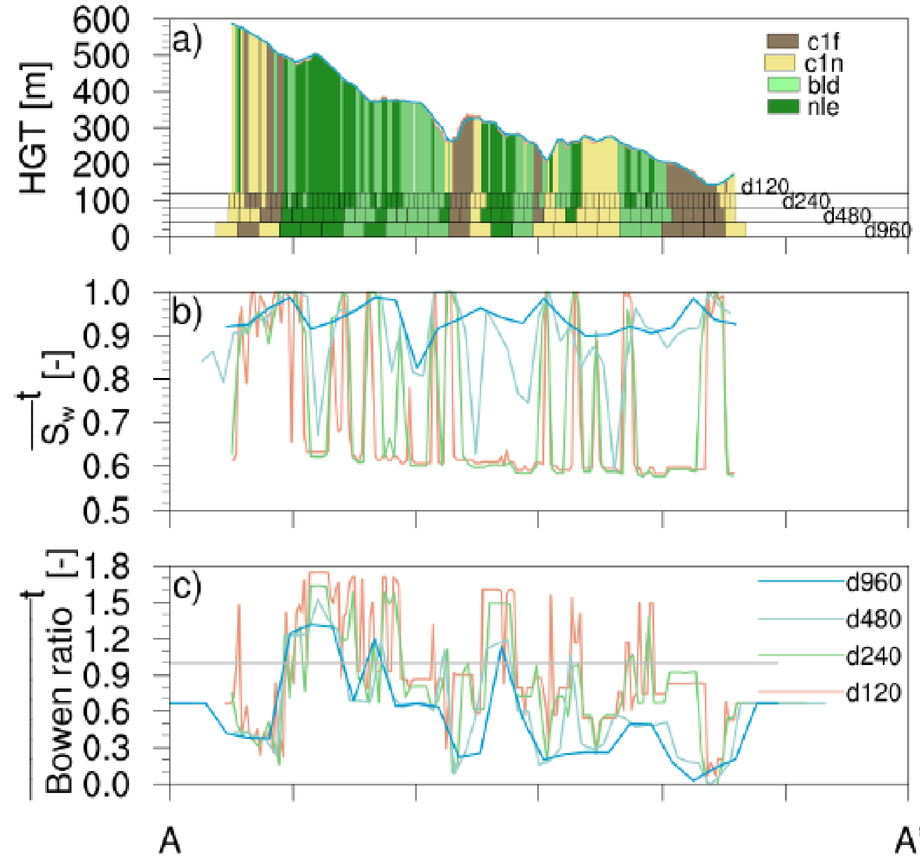


Table 4. Annual average Bowen ratio and standard deviation along the cross-section AA′ for the land-use classes nle (needleleaf evergreen tree), bld (broadleaf deciduous tree), c1n (crops with seasonal LAI), and c1f (crops with fixed LAI).

PFT	120 m	240 m	480 m	960 m
nle	1.56 ± 0.16	1.35 ± 0.22	1.22 ± 0.12	1.24 ± 0.07
bld	0.82 ± 0.08	0.72 ± 0.08	0.60 ± 0.09	0.59 ± 0.08
c1n	0.46 ± 0.13	0.50 ± 0.15	0.36 ± 0.13	0.28 ± 0.07
c1f	0.67 ± 0.28	0.53 ± 0.38	0.17 ± 0.11	0.18 ± 0.13

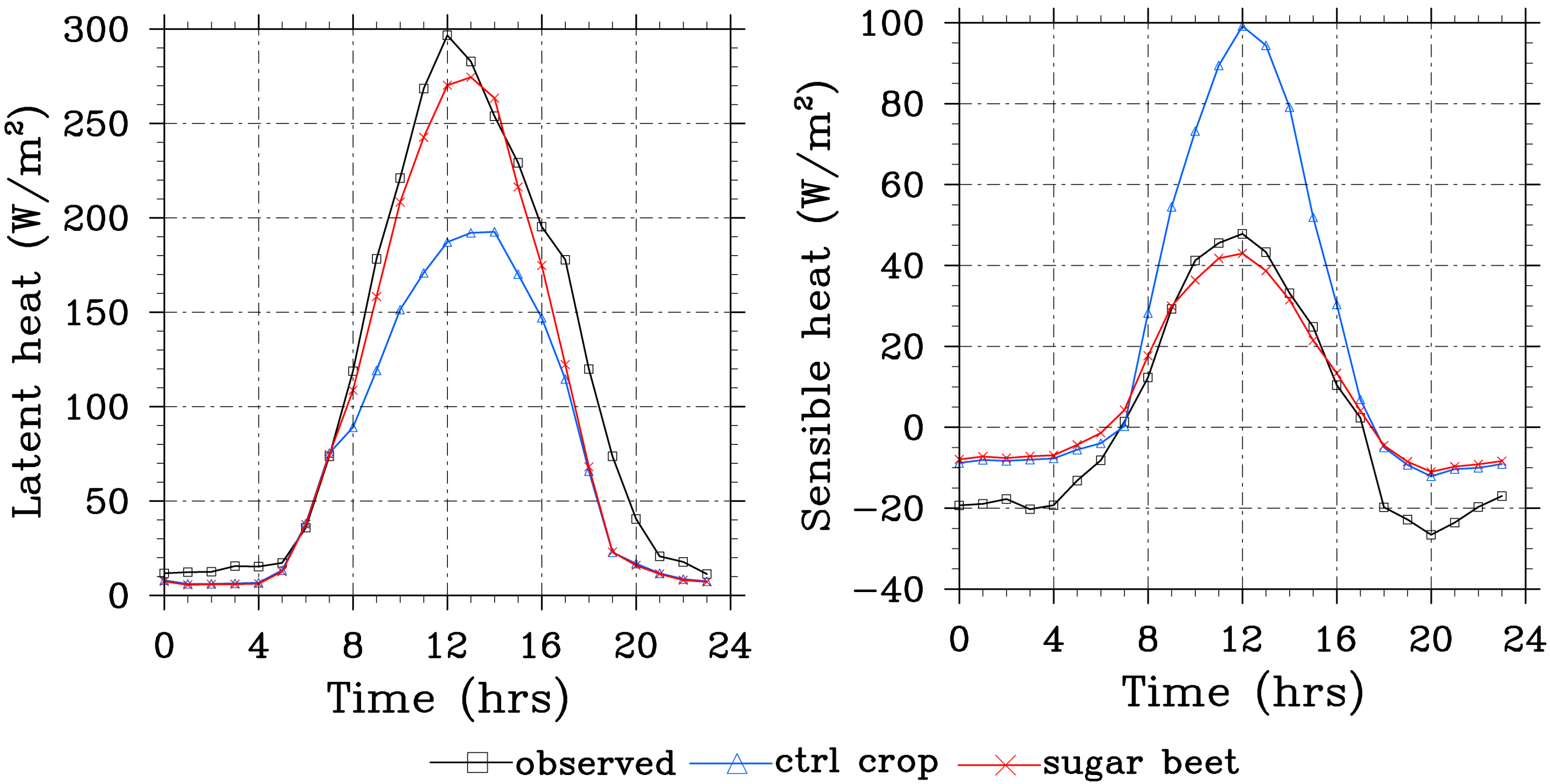
P. Shrestha et al. (2015, HESS)



- Non-local controls of soil moisture patterns by grid resolution (100-1000m res.)
- Strong modulation of soil temperature and surface fluxes by local PFTs
- Non-linear scaling behaviour of energy balance with respect to grid resolution

TerrSysMP sensitivity and improvements
Impact of plant-physiological parametrisations

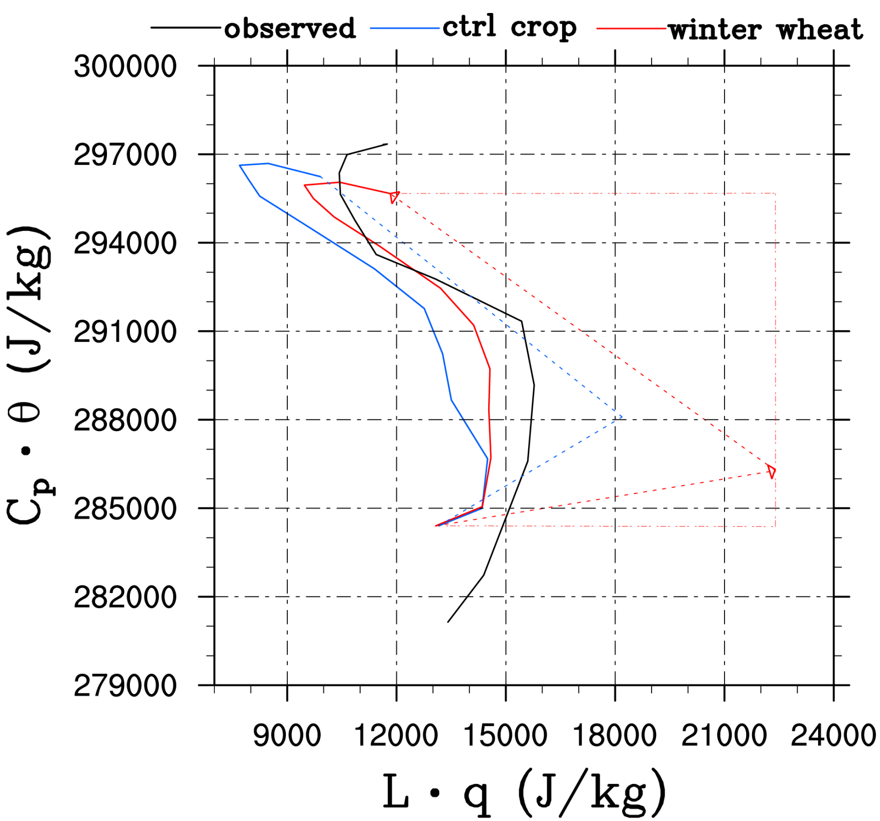
- Better photosynthesis reproduction (improvement of CLM in TerrSysMP): sign. influence on partitioning of fluxes, spatio-temporal variability of soil water, temperature and rate of carbon fixation
- Monthly averaged diurnal cycle, Selhausen site, June 2011 (TR32, NRW model domain)

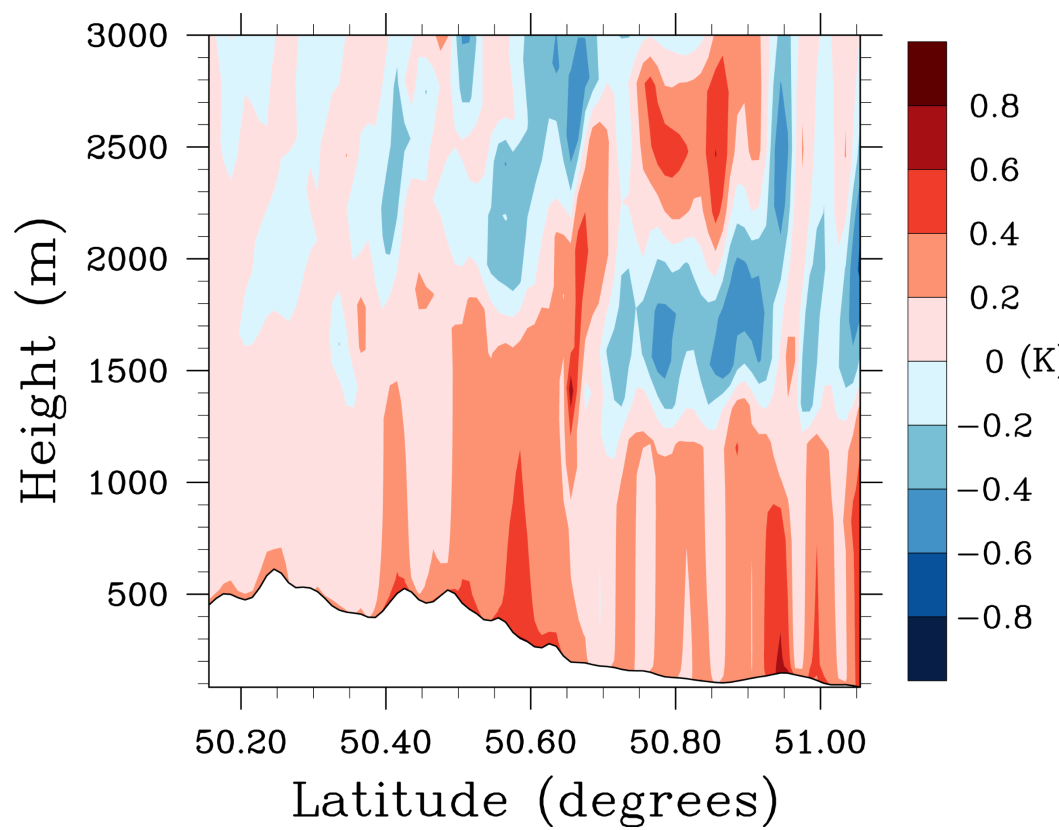


M. Sulis et al. (2014, J HYDROMETEOROL)

TerrSysMP sensitivity and improvements
Impact of plant-physiological parametrisations

- Impact on flux partitioning influences evolution of atmospheric boundary layer
- Semi-idealized L-A coupling experiment
- Mixing diagram for PBL energy balance evaluation; potential temperature difference, 2011-06-02

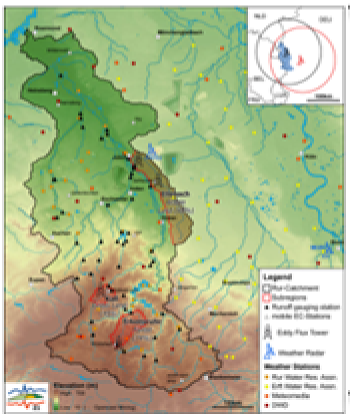




M. Sulis et al. (2014, J HYDROMETEOROL)

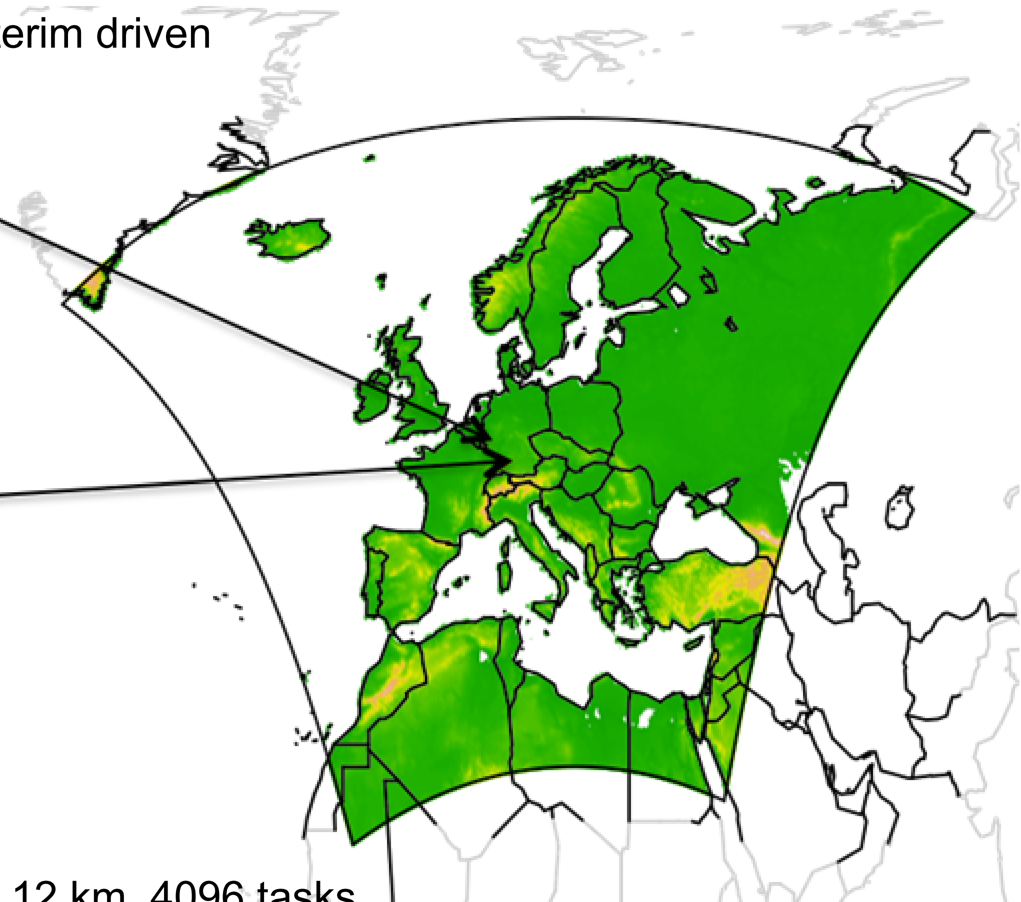
Water cycle, coupled European model domains
From catchment to continental scales

Multi-year hindcast study, ERA-Interim driven
Ongoing simulations



TR32

Shrestha et al., 2014,
Rahman et al., 2014, ...

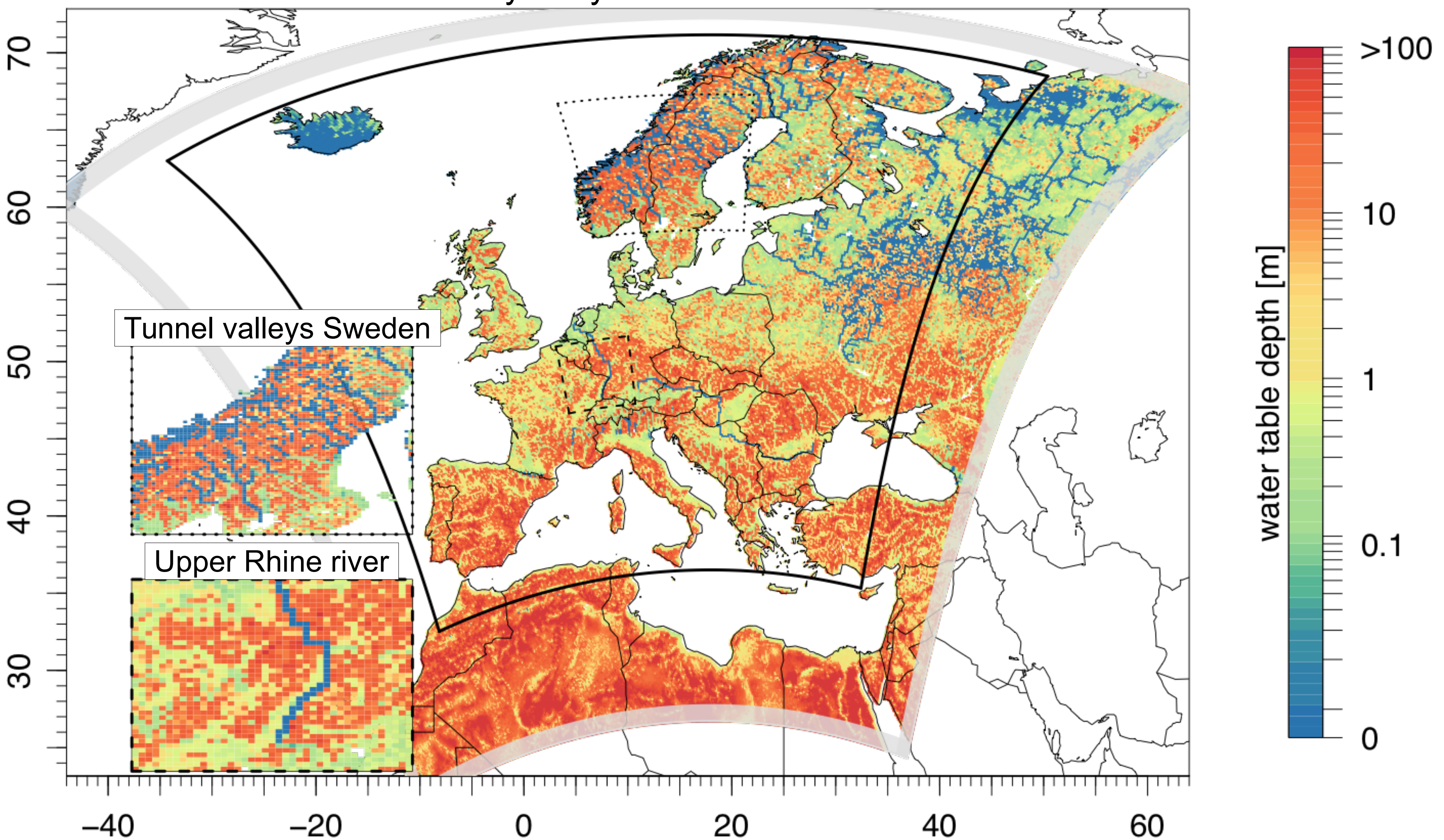


EURO-CORDEX EUR-11, about 12 km, 4096 tasks
Vertical levels: 50 (COSMO), 10 (CLM3.5), 15 (ParFlow)
Time steps: 60 s (COSMO), 1h (CLM3.5), 1h (ParFlow)
COSMO = 1680 tasks (42x40), CLM = 256 tasks (1x256), ParFlow = 2160 tasks (48x45)

J. Keune (Meteorological Institute, University of Bonn)

Water cycle, coupled European model domains Simulated water table depth (ParFlow), spinup runs

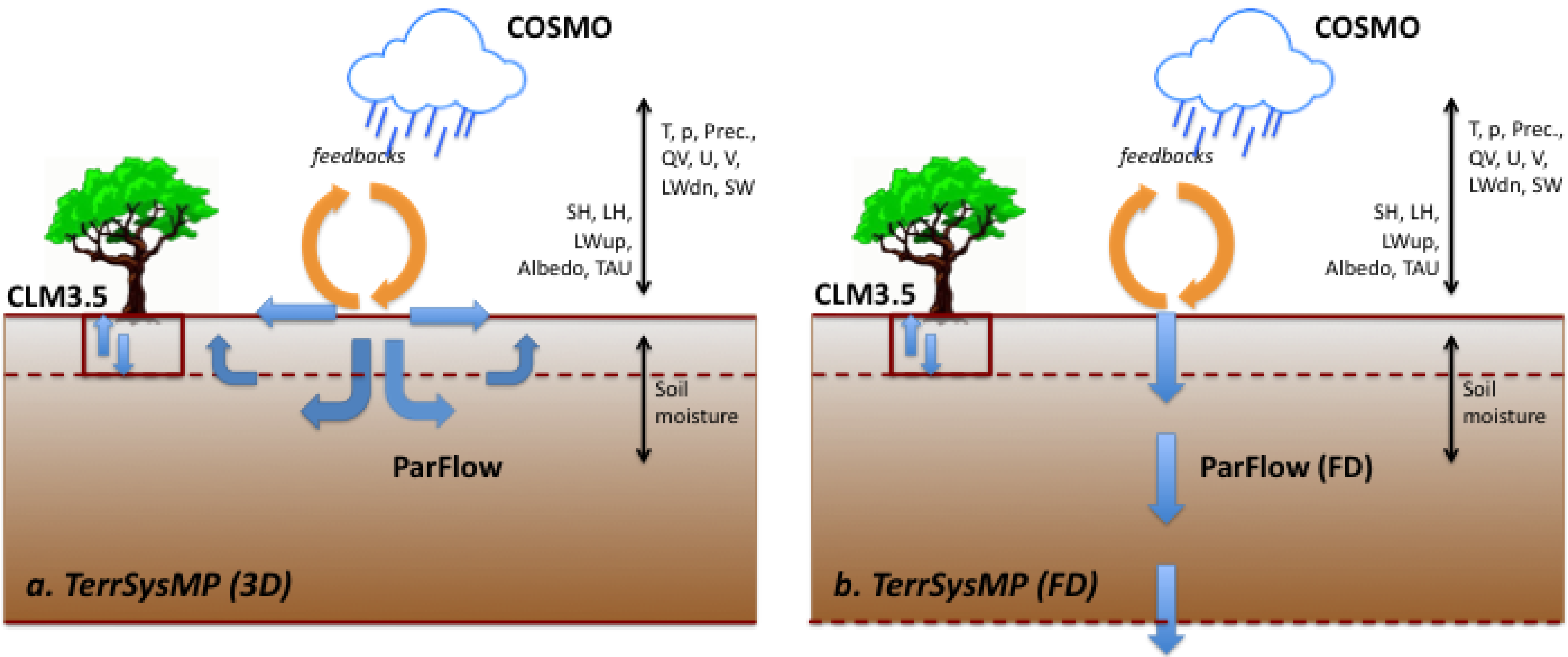
River networks start to evolve, redistribution of surface and groundwater in continuum approach
Surface runoff and subsurface hydrodynamics are linked



J. Keune (Meteorological Institute, University of Bonn)

Water cycle, effect of groundwater treatment 3D vs "free drainage" (ParFlow)

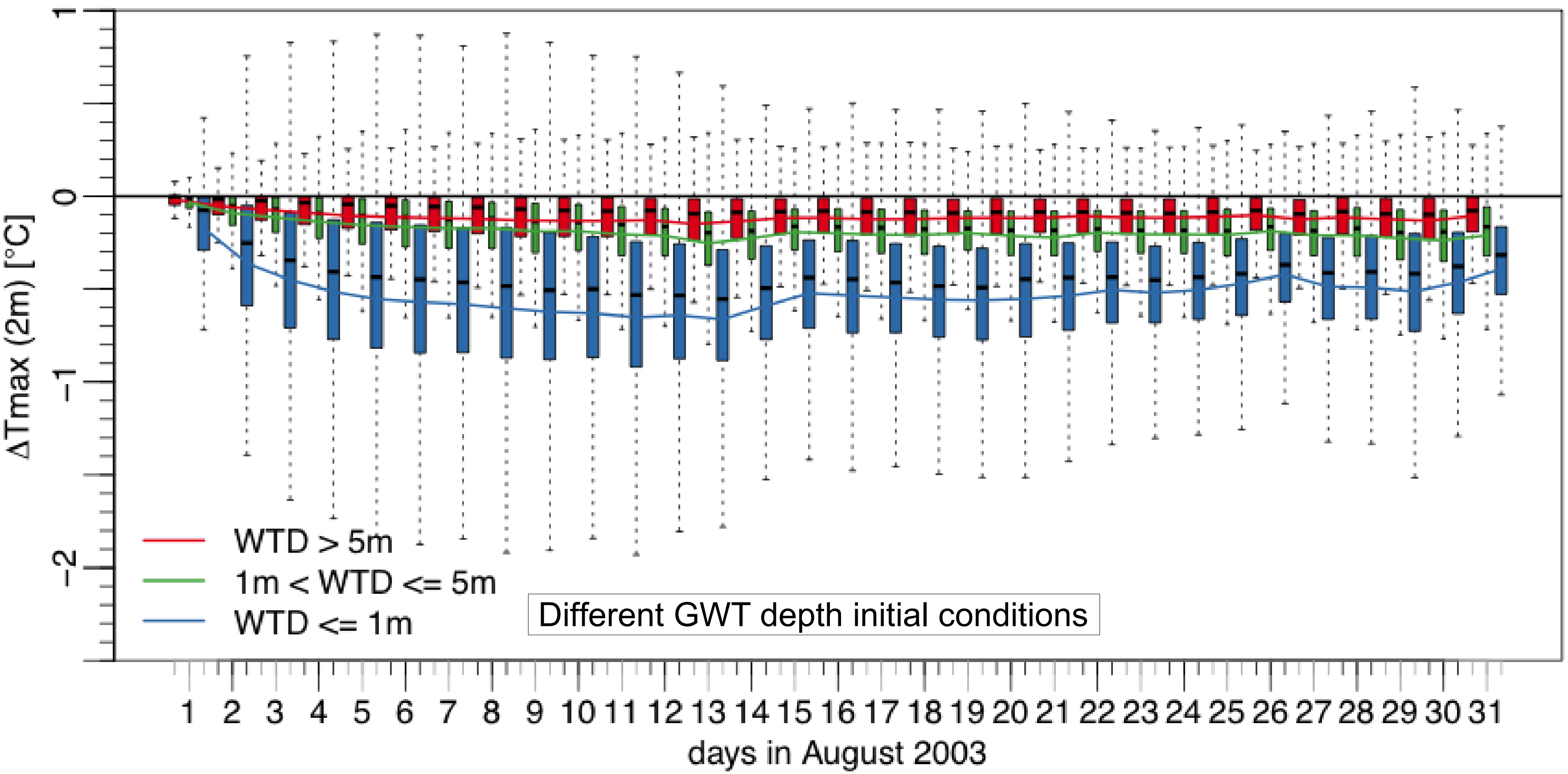
- Question: Impact of groundwater representation in regional climate simulations
- Land surface-atmosphere, subsurface-land surface, subsurface-land surface-atmosphere cpl.
- Hypothesis: Groundwater dynamics have significant impact on L-A feedbacks at continental scale



J. Keune (Meteorological Institute, University of Bonn)

Water cycle, coupled European model domains 3D-FD, August 2003 heatwave

- Simulation of heatwave 2003 with different physics-based 3D groundwater formulation and 1D free drainage approach, daily COSMO re-initialisation, transient ParFlow+CLM
- Daily maximum temperature difference over France; impact of groundwater configuration; lower temperature in 3D groundwater run, higher evaporative fraction (dual boundary layer concept)



J. Keune (Meteorological Institute, University of Bonn)

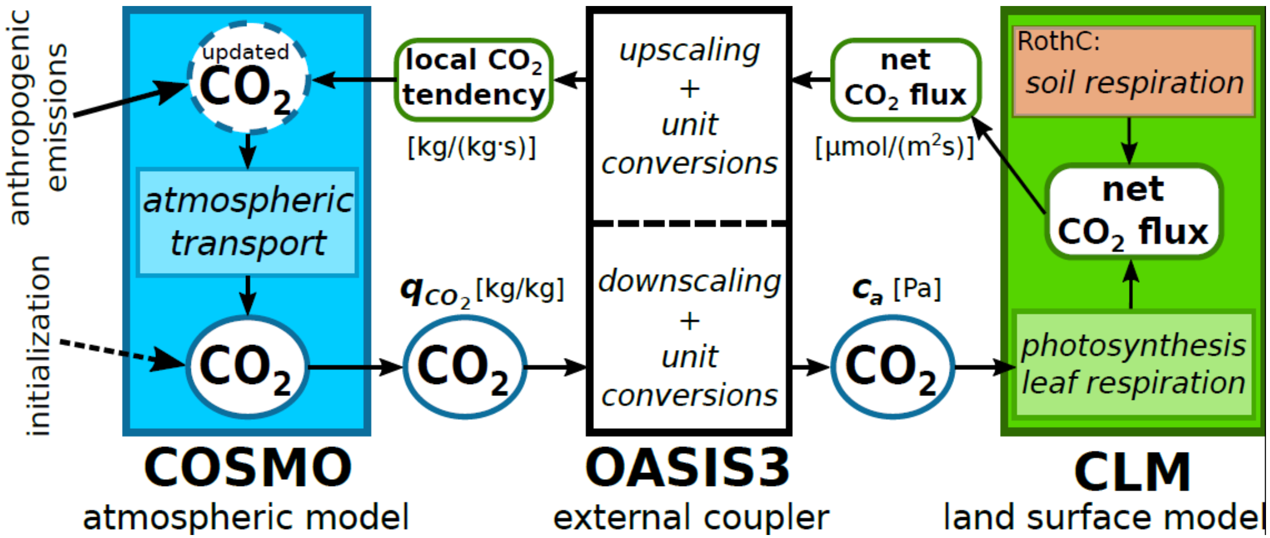
Further technical developments

TerrSysMP_CO2

TerrSysMP-PDAF

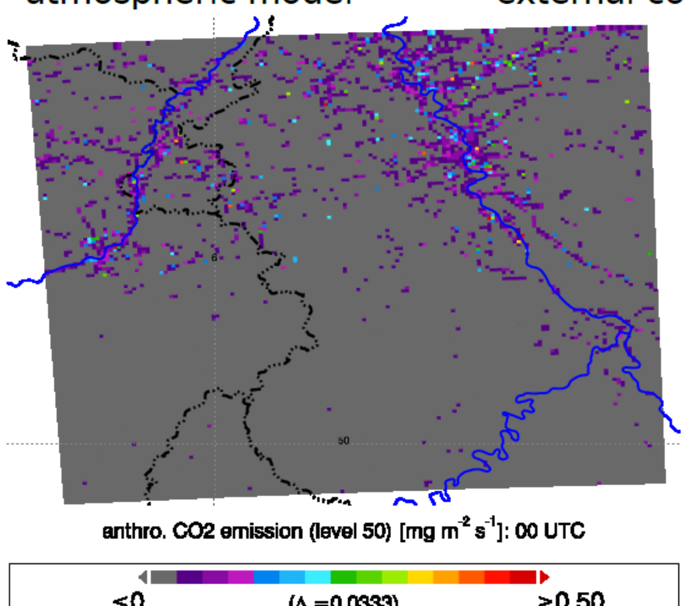
Monitoring runs

TerrSysMP_CO2
Inclusion of CO2 coupling in TerrSysMP



CO_2 added as a prognostic variable in COSMO
Source terms of CO_2 added in CLM
Two-way coupling

CO2 initialisation in COSMO
COSMO sfc lvl CO2 → CLM
CLM: natural CO2 fluxes
COSMO ← CLM CO2 tend.



Anthropogenic CO2 emissions as source Terms for COSMO

Typical diurnal cycle

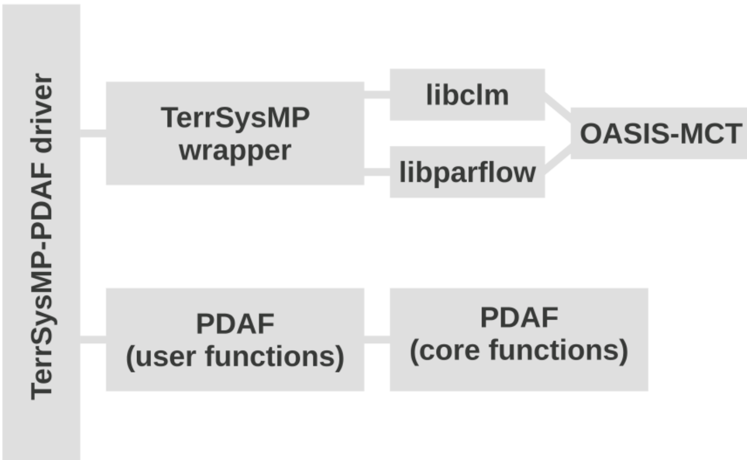
NRW model domain
1 km resolution

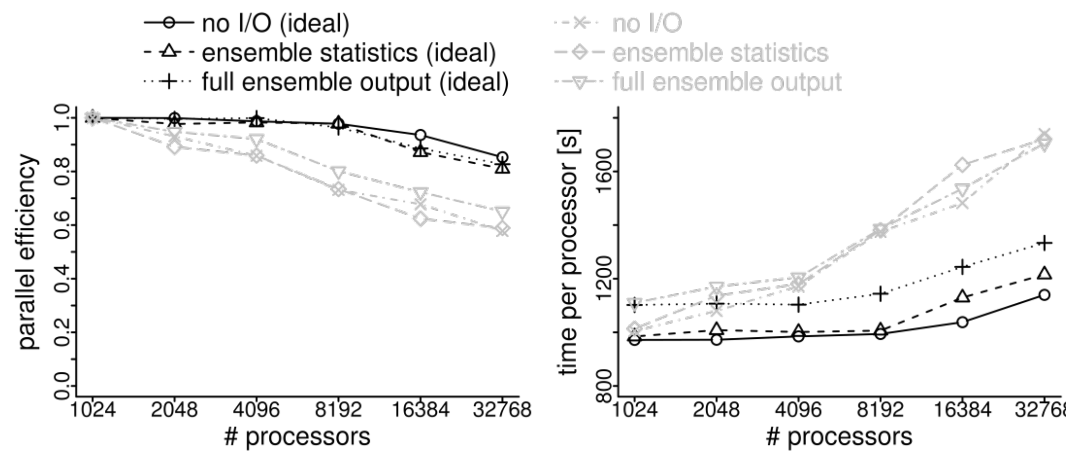
Natural fluxes: plant types, soil conditions (photosynthesis and respiration)
Anthropogenic emissions

Net ecosystem exchange and transpiration are sensitive to CO2:
Atmospheric CO2 impacts water and energy fluxes

M. Übel (Meteorological Institute, University of Bonn)

TerrSysMP-PDAF
Implementation of parallel data assimilation framework



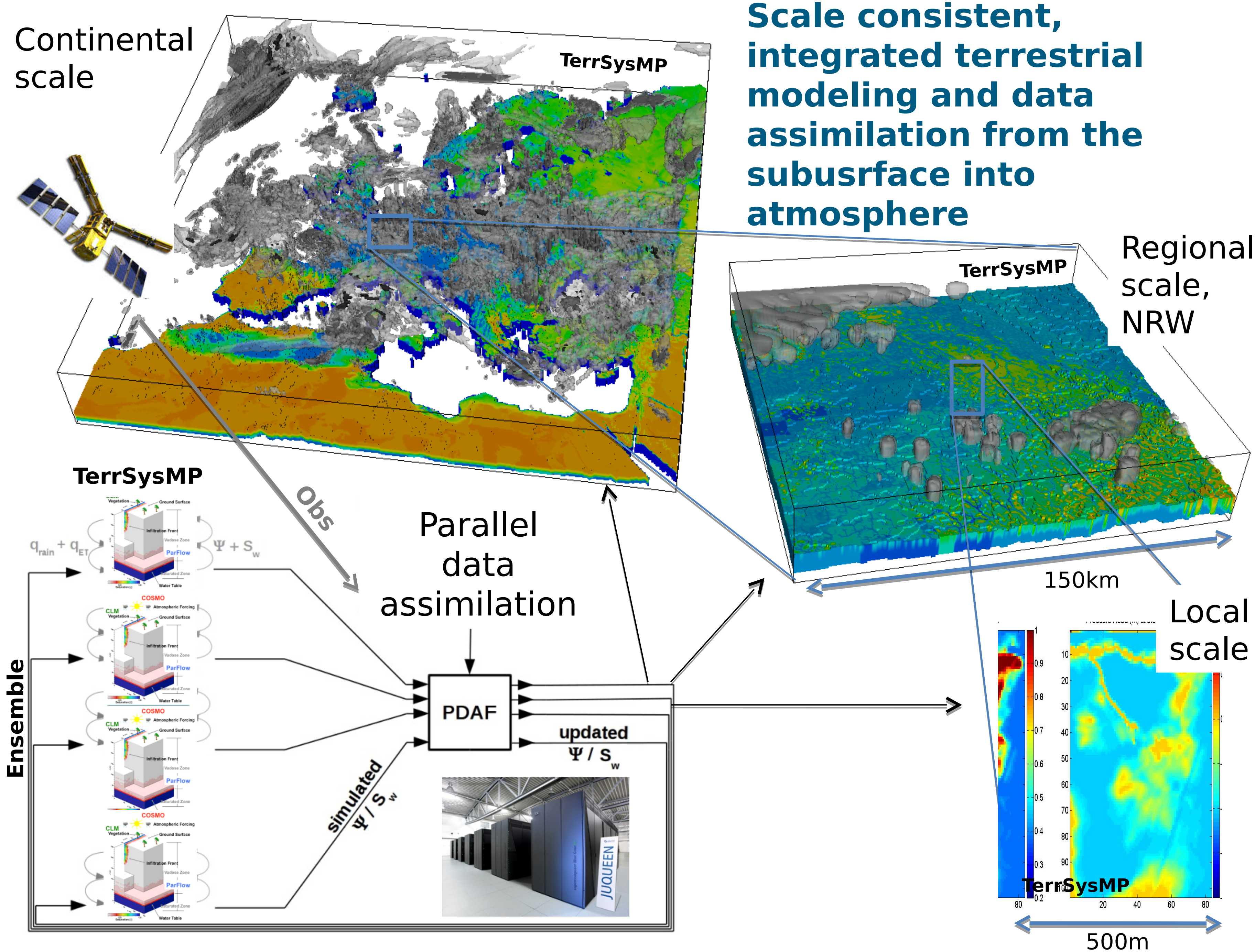


- TerrSysMP coupled with Parallel Data Assimilation Library (PDAF from AWI)
- Currently implemented for land surface-subsurface part; COSMO integration is on the way
- Keeps modularity of TerrSysMP
- Fully parallel; good scalability
- Assimilation of pressure (GW-levels, discharge) and soil moisture data
- Parameter update: Saturated hydraulic conductivity, Manning's coefficients, Texture
- Currently EnKF is implemented; additional filters are available in PDAF

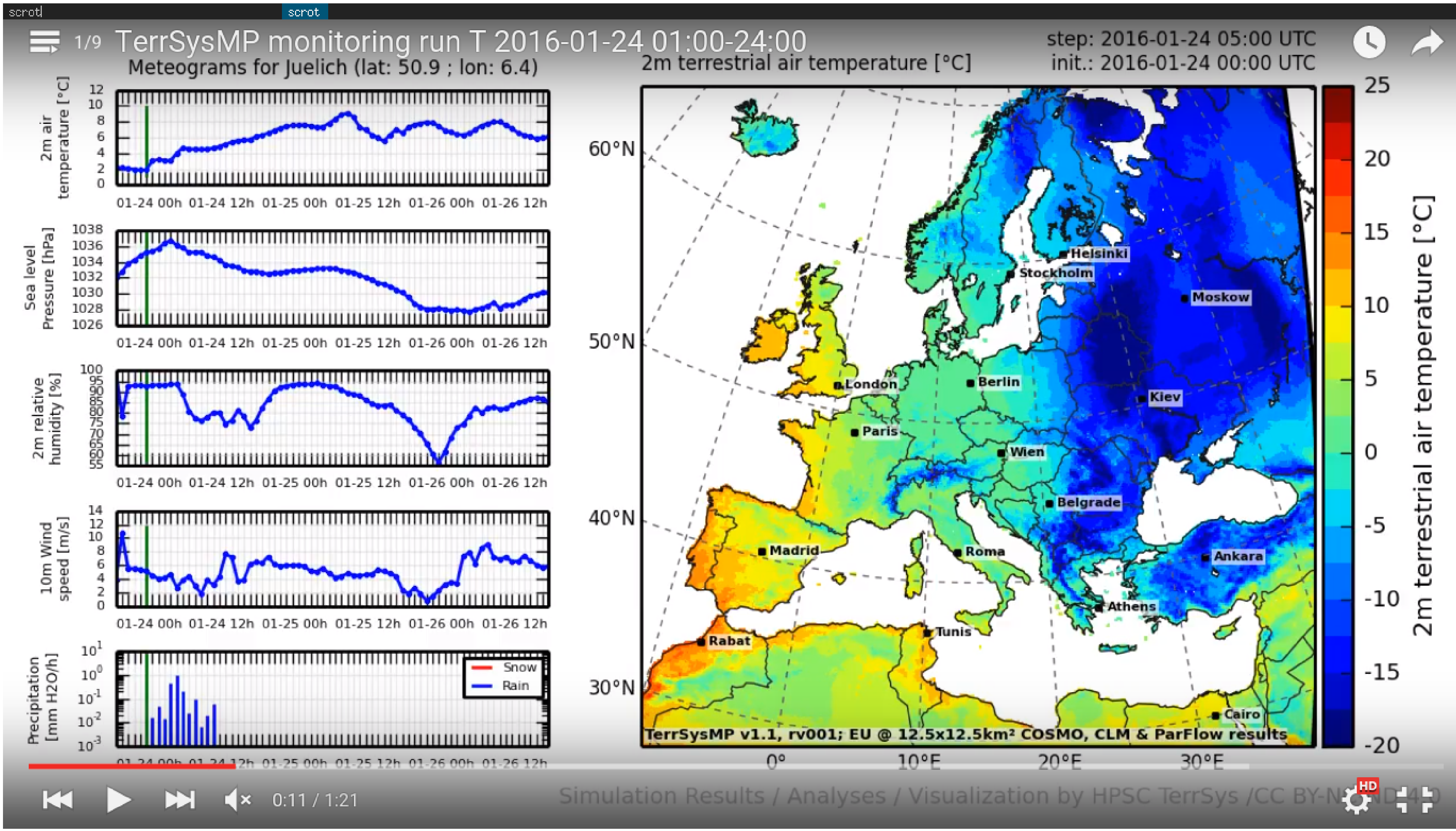
W. Kurtz et al. (GMDD)

Possibilitiy for water cycle monitoring

Scale consistent, integrated terrestrial modeling and data assimilation from the subusrface into atmosphere

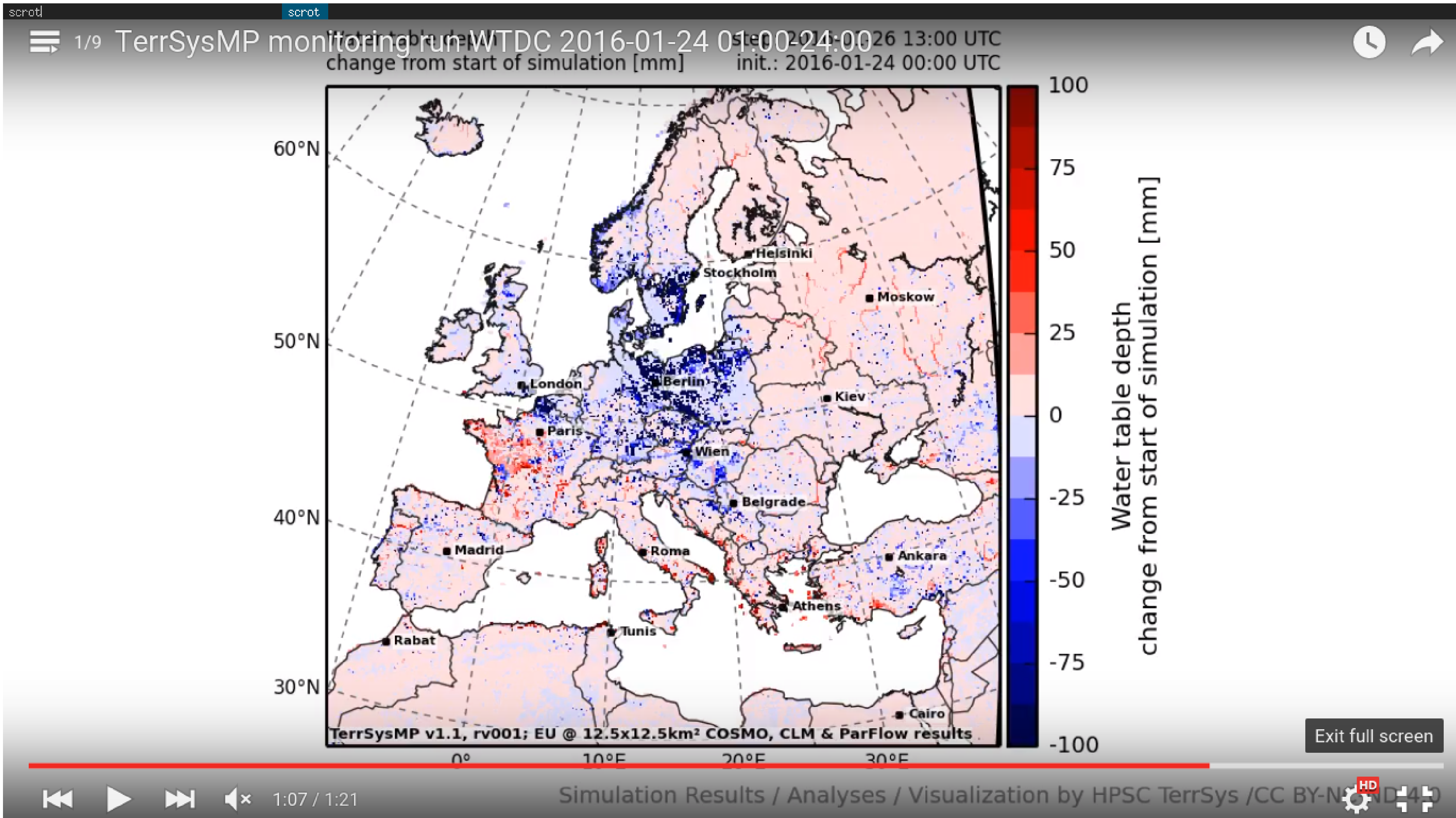


Nighlty monitoring runs (JSC/JURECA)
Fully coupled TerrSysMP: Europe EUR-11 12km



JÜLICH
FORSCHUNGSZENTRUM

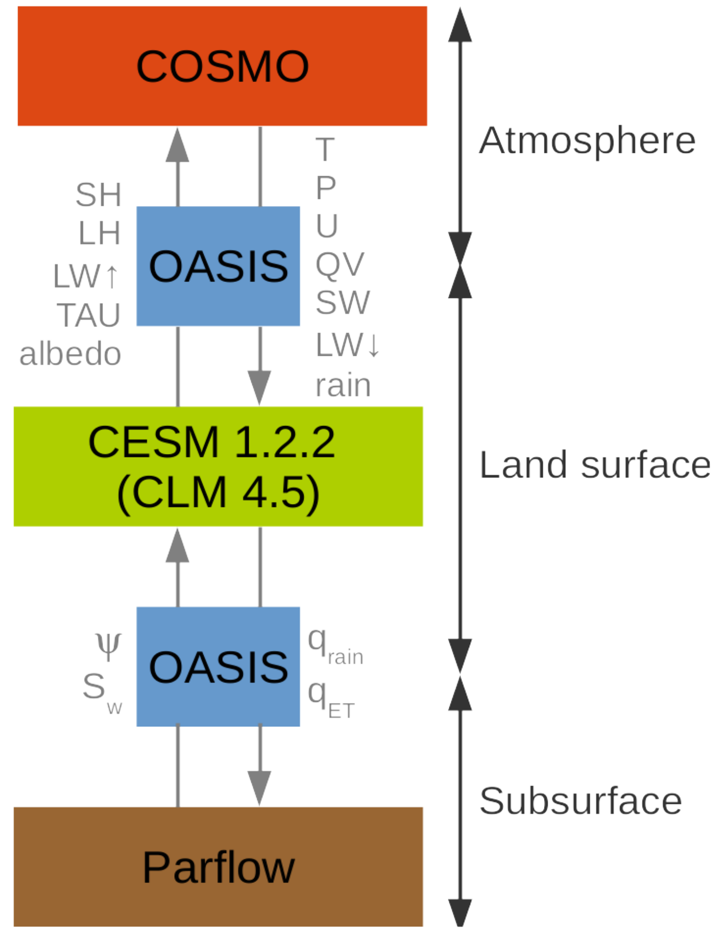
Nighlty monitoring runs (JSC/JURECA)
Fully coupled TerrSysMP: Europe EUR-11 12km



Summary and outlook

Summary and outlook
Towards “earth system modell at regional scale”

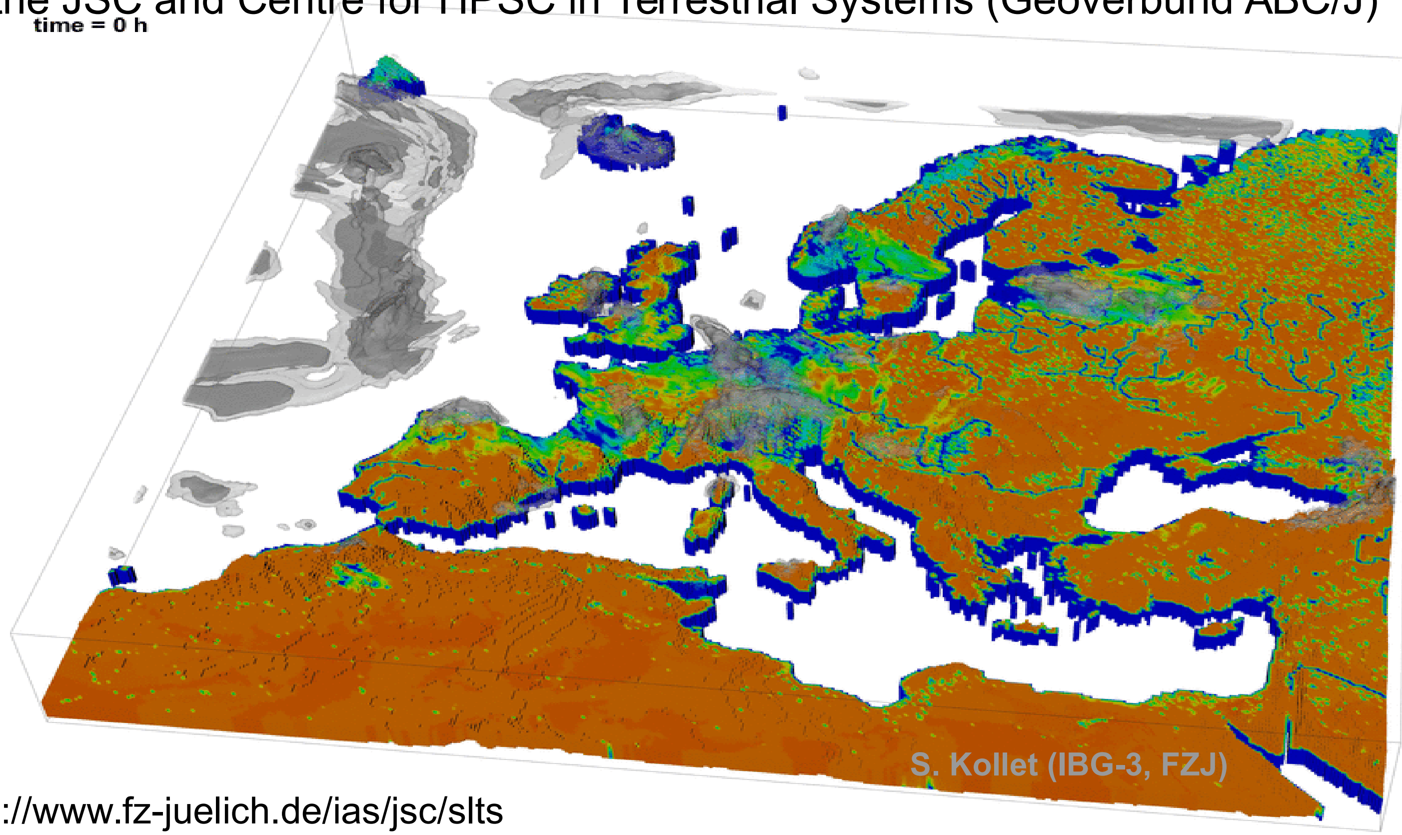
- TerrSysMP allows for a physically consistent desciption of interactions between compartments of geo-ecosystem accross spatial and temporal scales
- Detailed reproduction of water cycle processes
- Towards continental domains
- Climate change projections (at high resolution)
- LES simulations
- Work on understanding of implications of coupling
- Technical developments and optimisations
  - Flexible coupling design
  - Improved spinup of subsurface component
  - CLM4.5, COSMO5.0, GPU COSMO, ICON
  - Use of accelerators (GPUs or MICs)
  - Big data: parallel I/O, in-situ processing
  - Ocean?



G. He, W. Kurtz (IBG3, FZJ)

SimLab TerrSys

of the JSC and Centre for HPSC in Terrestrial Systems (Geoverbund ABC/J)



3 day snapshot
Elbe flood event
May/June 2013

http://www.fz-juelich.de/ias/jsc/slts

http://www.hpsc-terrsys.de

http://www.geoverbund-abcj.de

Follow us on Twitter @HPSCTerrSys

YouTube channel: HPSC TerrSys