



Z04: Central Supercomputing Support

Enabling DETECT through HPC

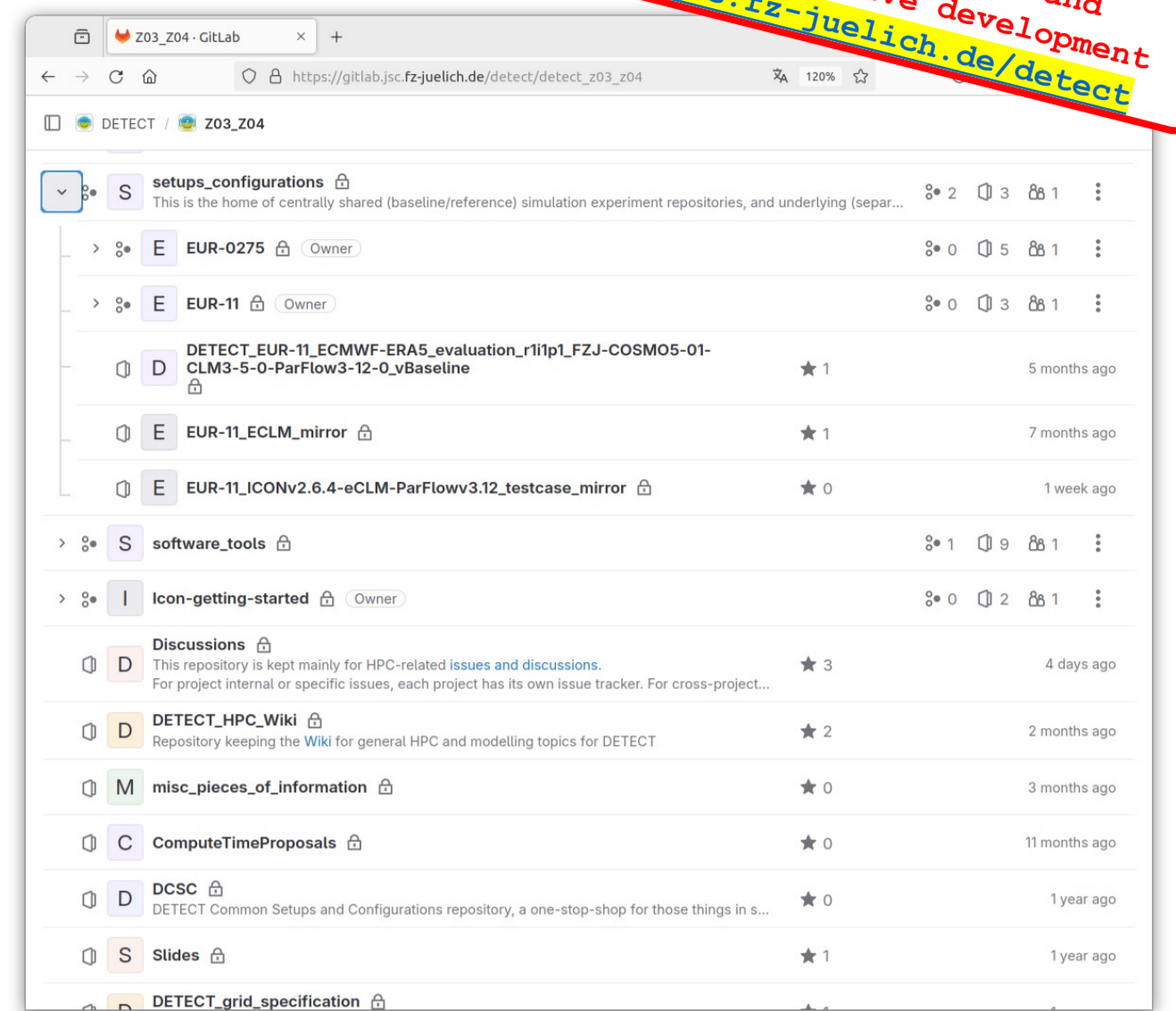
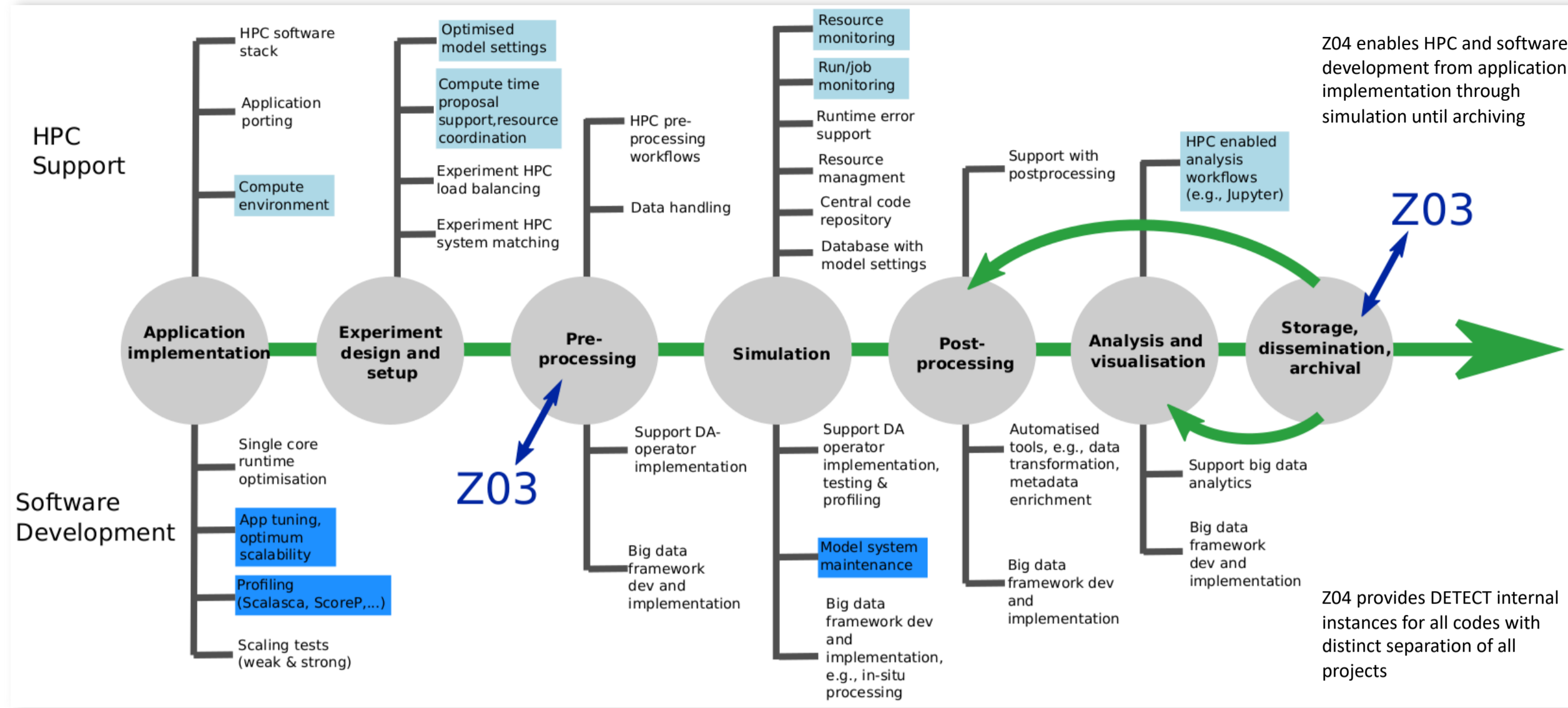
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with special support from Paul Rigor^{1,4}, Niklas Wagner*, Carl Hartick*, and others

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Introduction, Z04 objectives and tasks

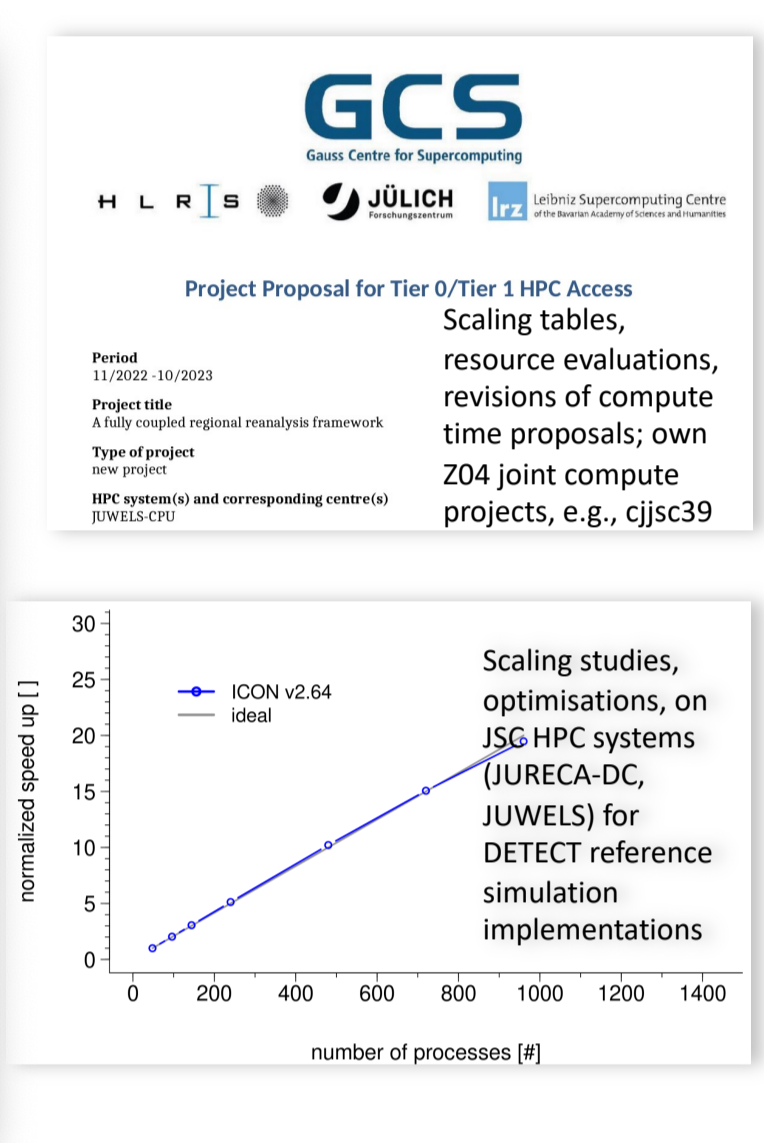
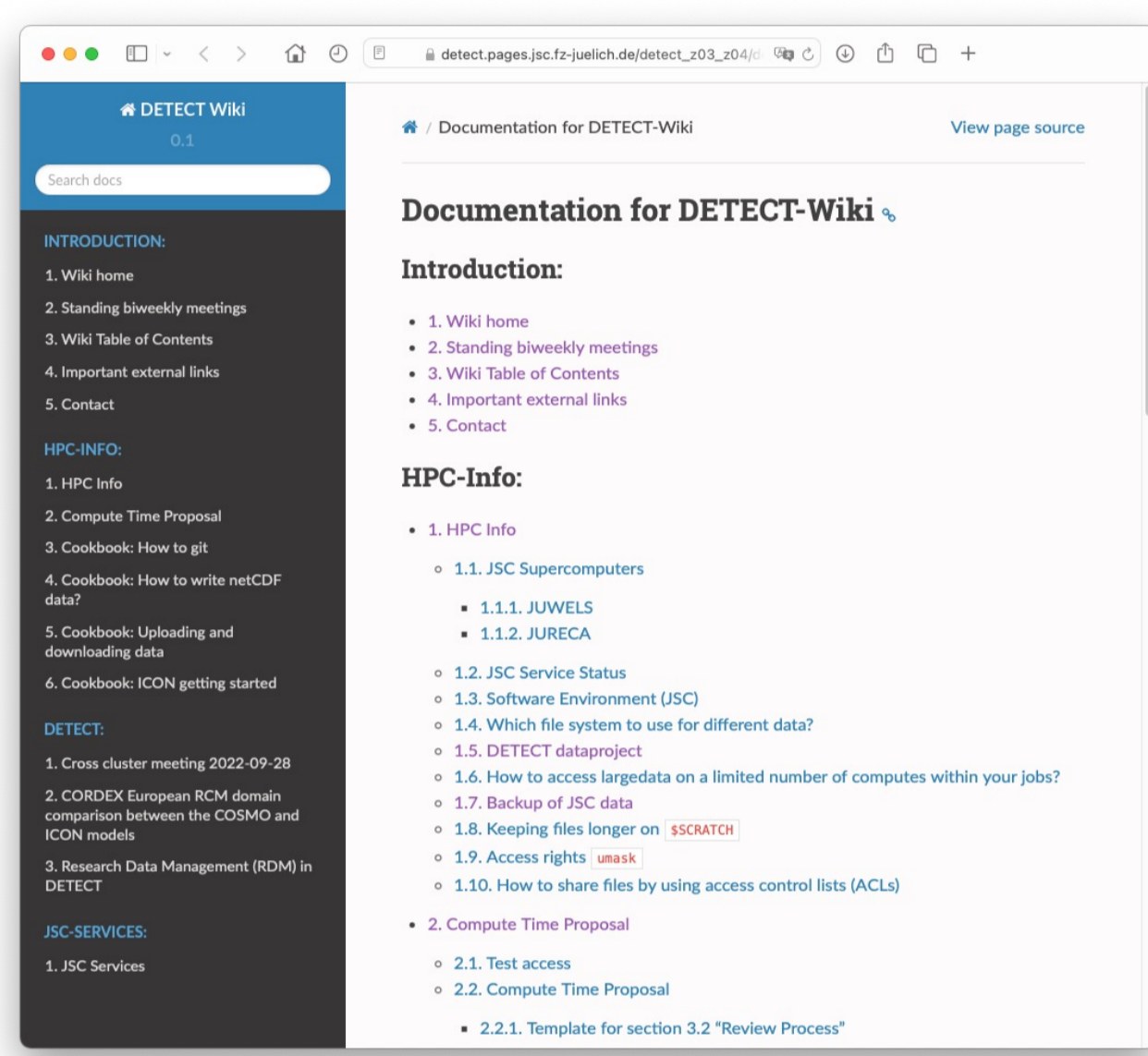
- Our objectives:
 - Support the CRC to conduct its numerical model and simulation experiments, as well as processing and analysis tasks in a big data context
- Our tasks in relation to the entire CRC – in close synchronisation with Z03 (INF):
 - Basic support for a multitude of HPC-related issues (porting and tuning of scientific software applications, like simulation, processing, analysis, and visualization codes, on the latest supercomputers (JSC, UB HPC/A-Lab)
 - Help with development (models, analysis and processing tools, workflows), support performance optimizations, towards big data readiness (Z03 links)
 - Simulation support as a service to the CRC (common setups and configurations, provenance tracking and configuration management, reproducibility)
 - Training of early-career scientists at the interface of geoscience, HPC, and data science, maintain a regular support infrastructure



most central tool for reproducible, versioned information exchange and management and collaborative development
<https://gitlab.jsc.fz-juelich.de/detect>

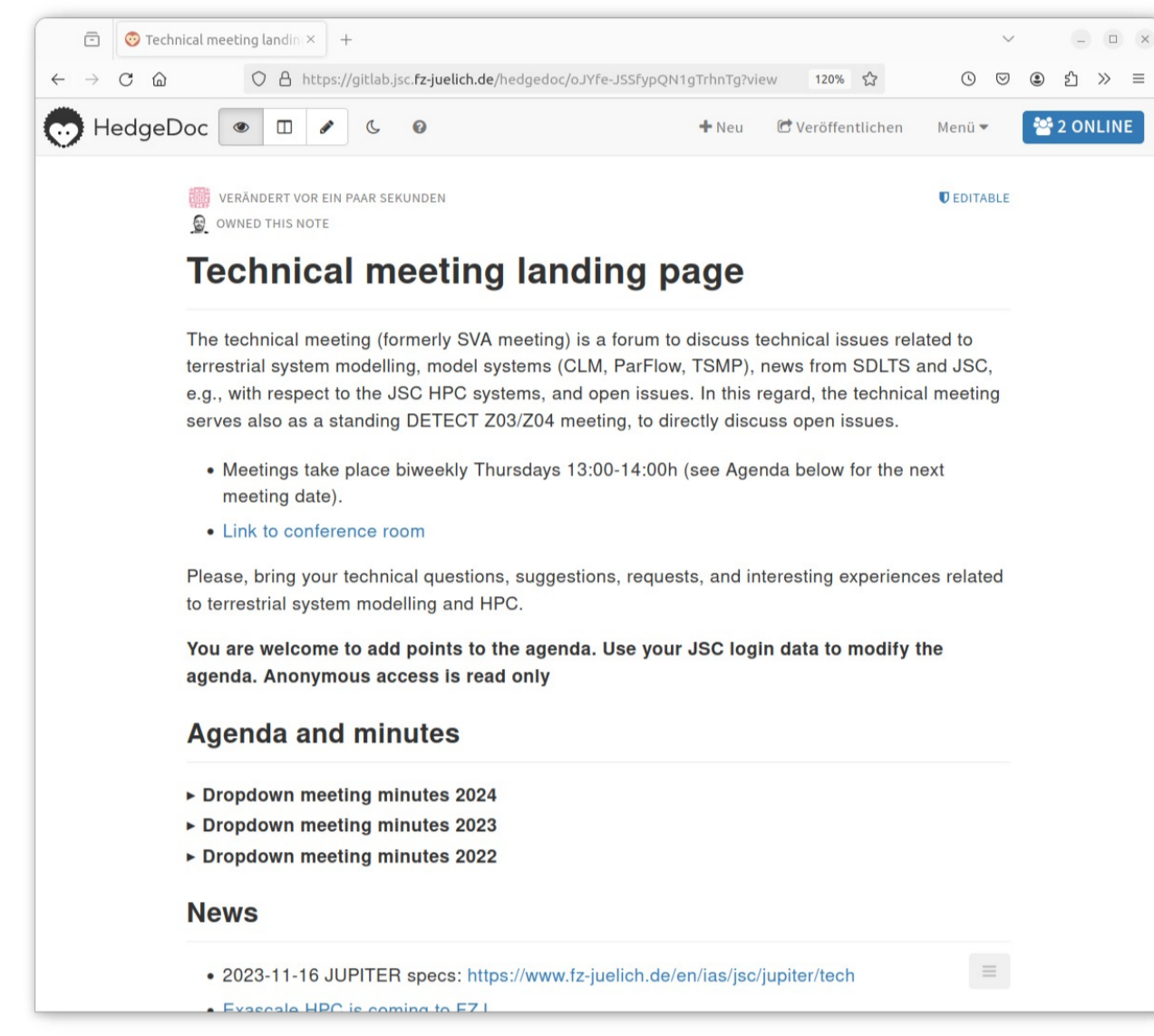
Basic HPC (and big data handling) support

- Information management via central DETECT GitLab
- Deployment and maintenance of HPC wiki pages
- Operation and moderation of issues and discussion board
- JSC compute time application support
- Code porting to JSC HPC systems
- Enabling parallel computing
- Software environments at JSC
- Data formats, meta data (CF)
- Conventions, standards (CMOR)



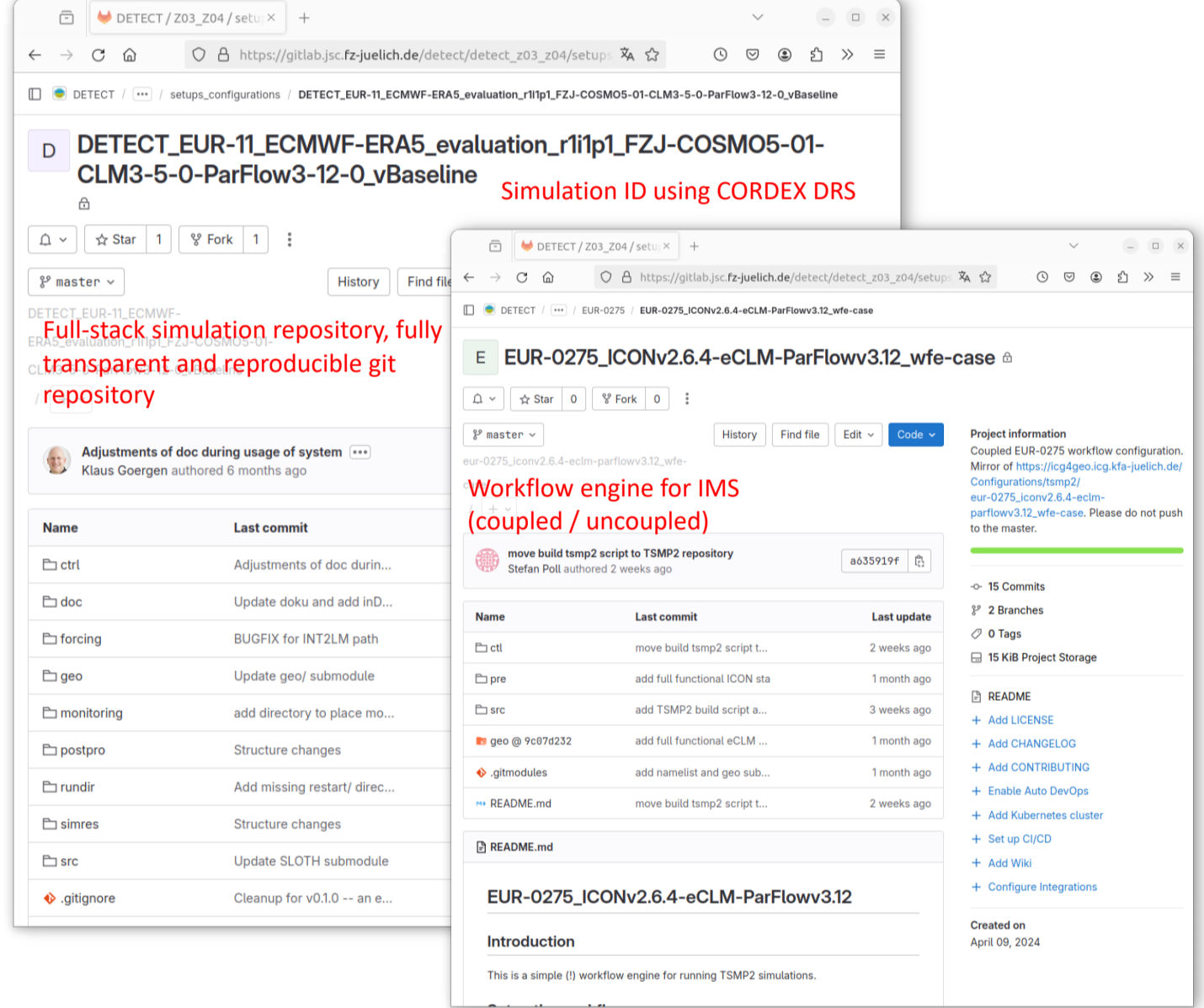
Regular meetings, part of DETECT training schemes

- Bi-weekly technical meetings, supporting all HPC matters, optional hackathon-style joint problem solving and development on site thereafter
- IRTG HPC training day for early-career DETECT staff
- HPSC TerrSys Fall School, week-long training on HPC and terrestrial system modelling



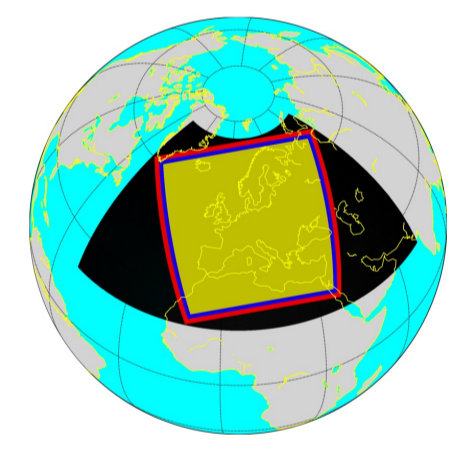
Simulation support, maintenance, coordination

- Model system maintenance (bug fixes, documentation, code adjustments, porting to latest HPC systems); via github (<https://github.com/HPSCTerrSys>), DETECT GitLab
- Supported coupled model systems: TSMP v1.x (COSMO+CLM+ParFlow), v2.x (ICON+eCLM+ParFlow)
- Profiling, tuning (e.g., I/O strategies), load balancing
- Preparation of forcing data, preparation of static fields (joint DETECT LULSC, LAI, hydrogeology, etc. datasets)
- Help with very large, long simulations (climate runs, convection permitting, ensembles)
- Custom workflow developments and optimisations
- Implementation of typical processing tasks
- Liaison and contribution to CORDEX-CMIP6 and CLMcom



Model system setups and configurations, intl. links

- DETECT Common Setups and Configuration (DCSC) framework: synchronize data flowpaths simulations (efficiency, hypothesis testing)
- Reference implementations: Unified configurations, setups, forcing data, model grids; data reference syntax, controlled vocabularies, variable lists

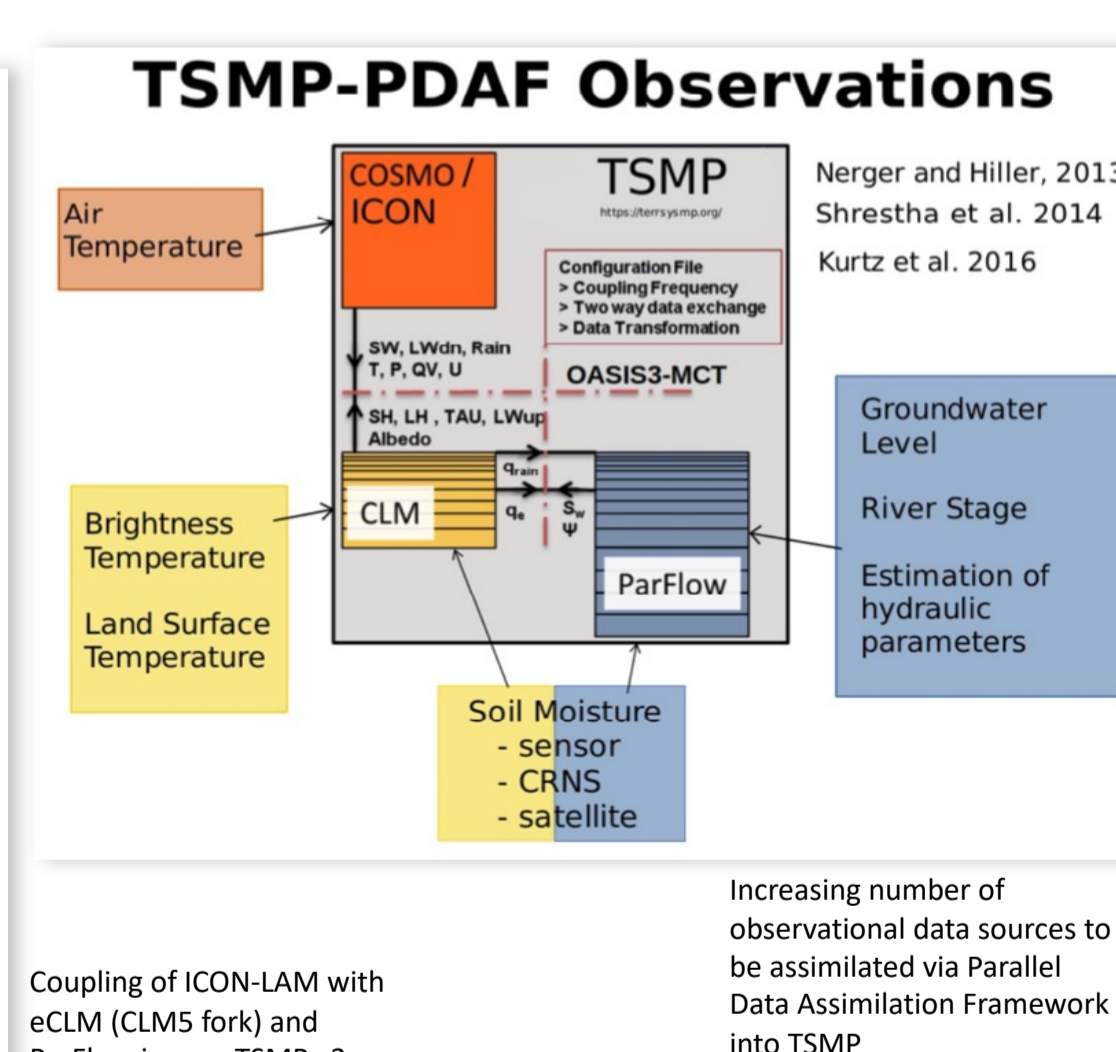
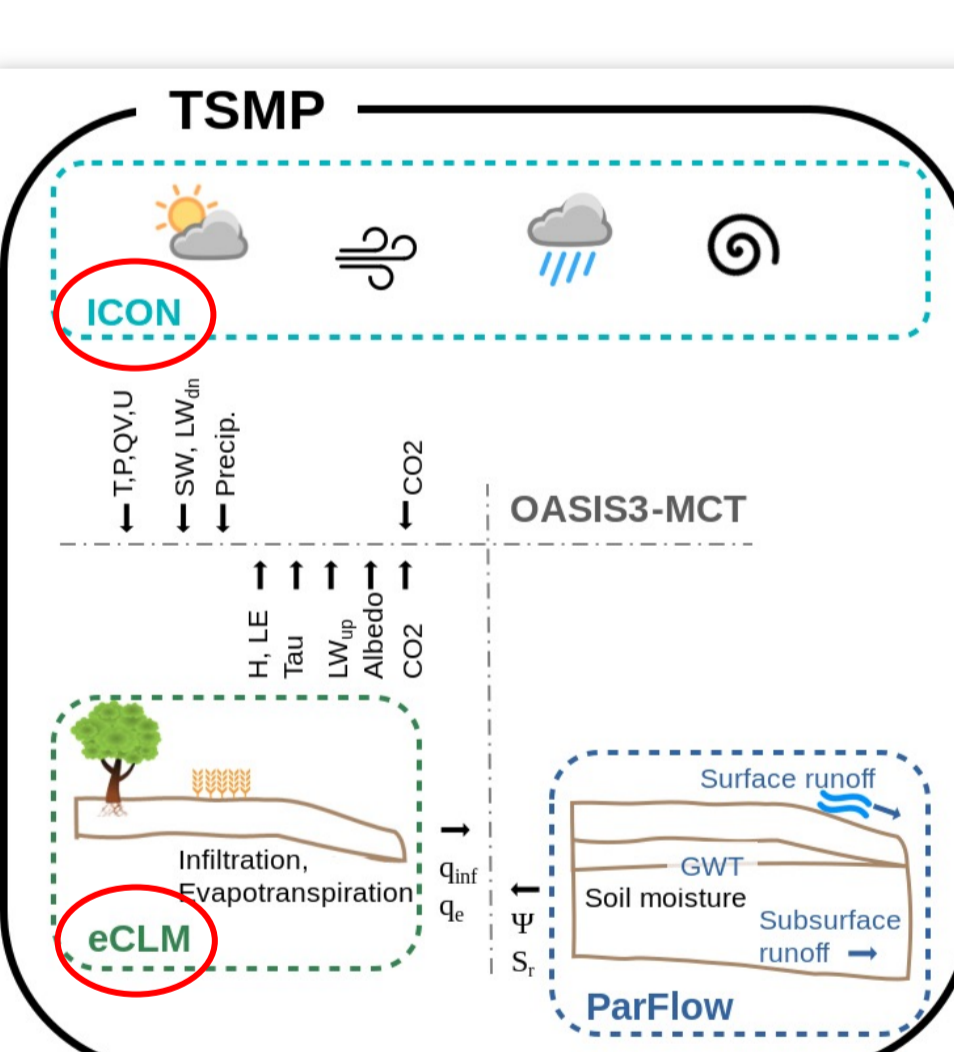
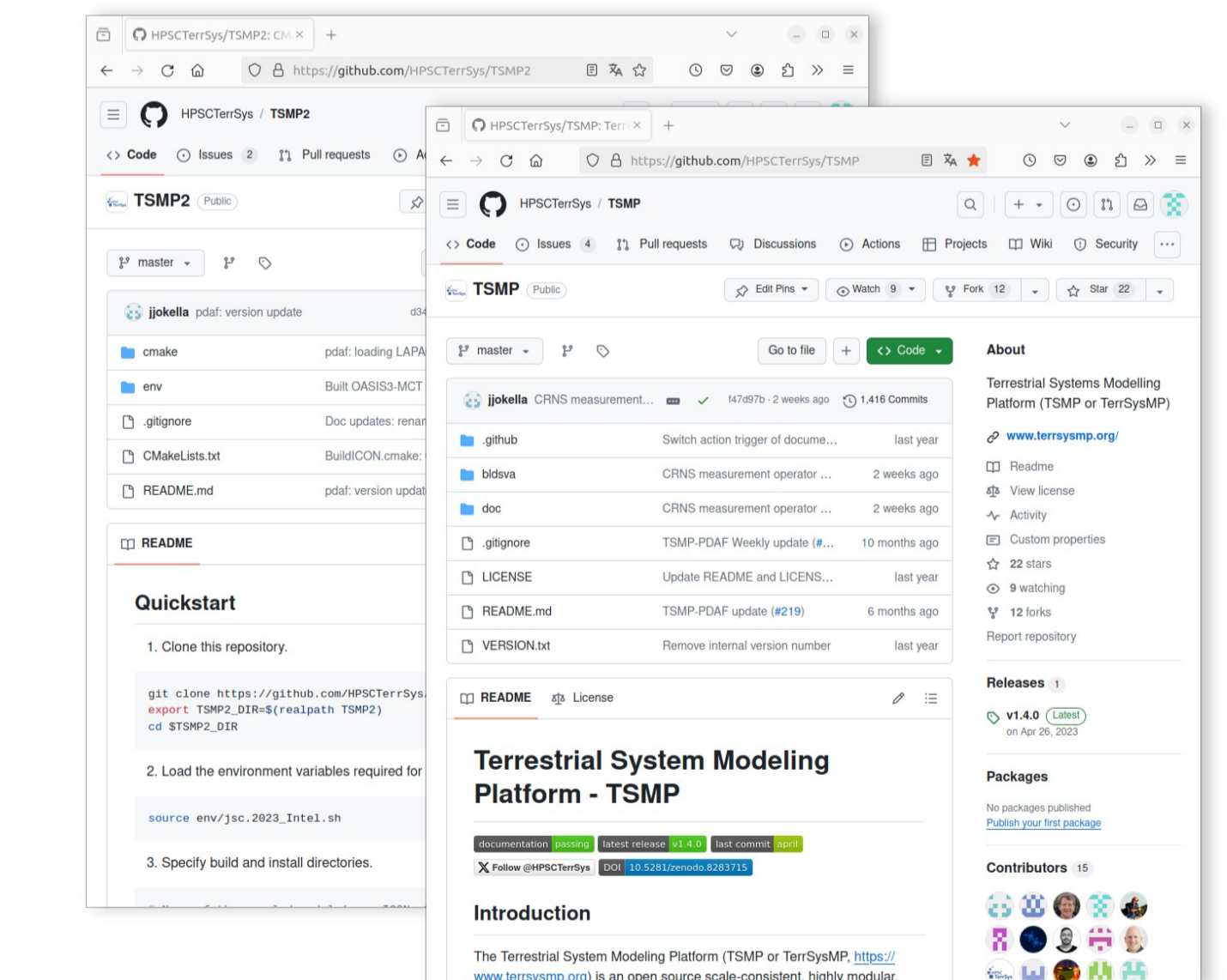


Regular lon-lat, rotated / curvilinear (EUR-11, EUR-0275), triangular (R13805, R13807) reference grids for standard (about 10-12 km) and convection-permitting resolutions (1-3 km)

TSMP2 (ICON+eCLM+ParFlow) – support of and involvement in all aspects of simulation experiments

Maintenance and development tasks around TSMP2:

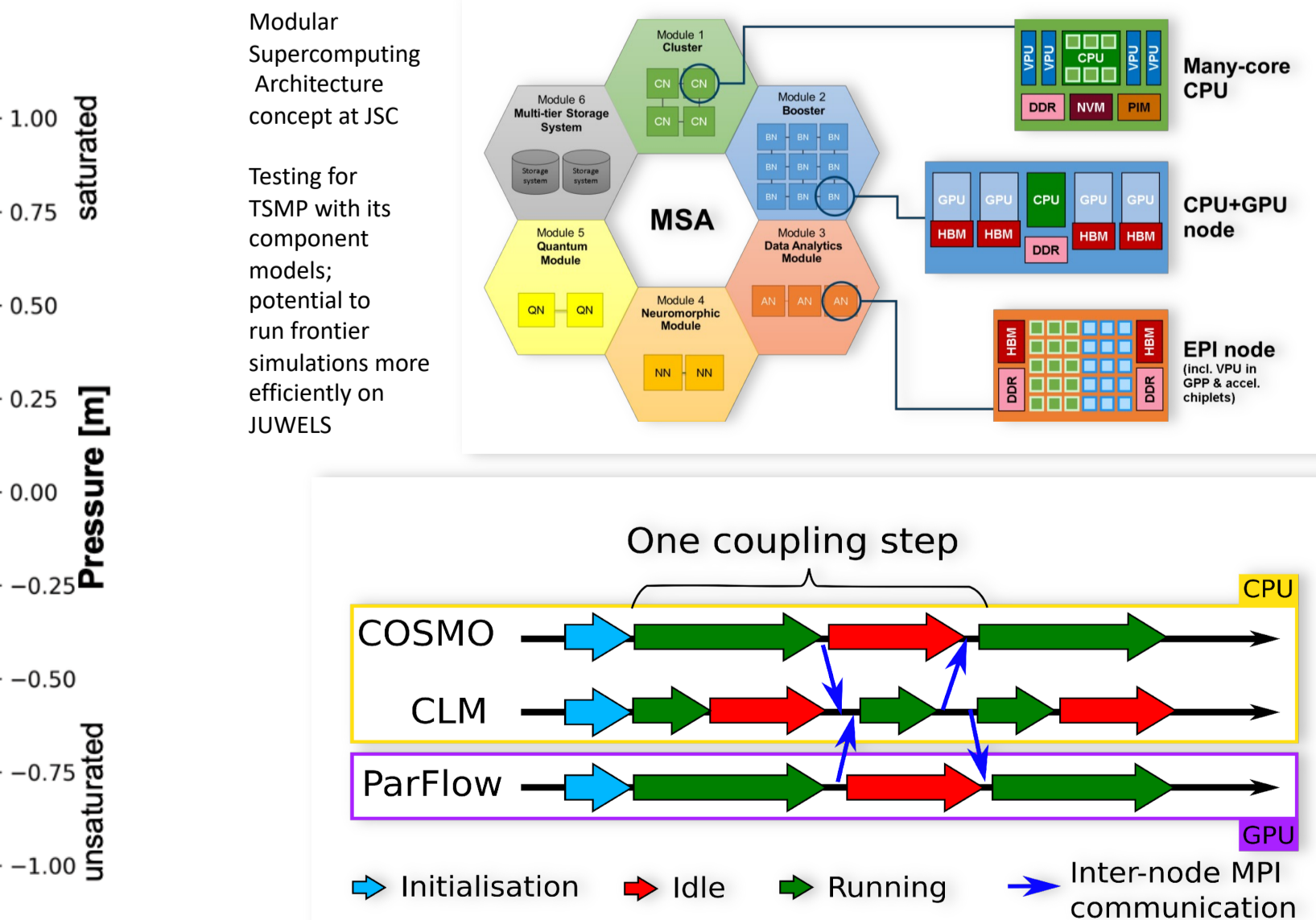
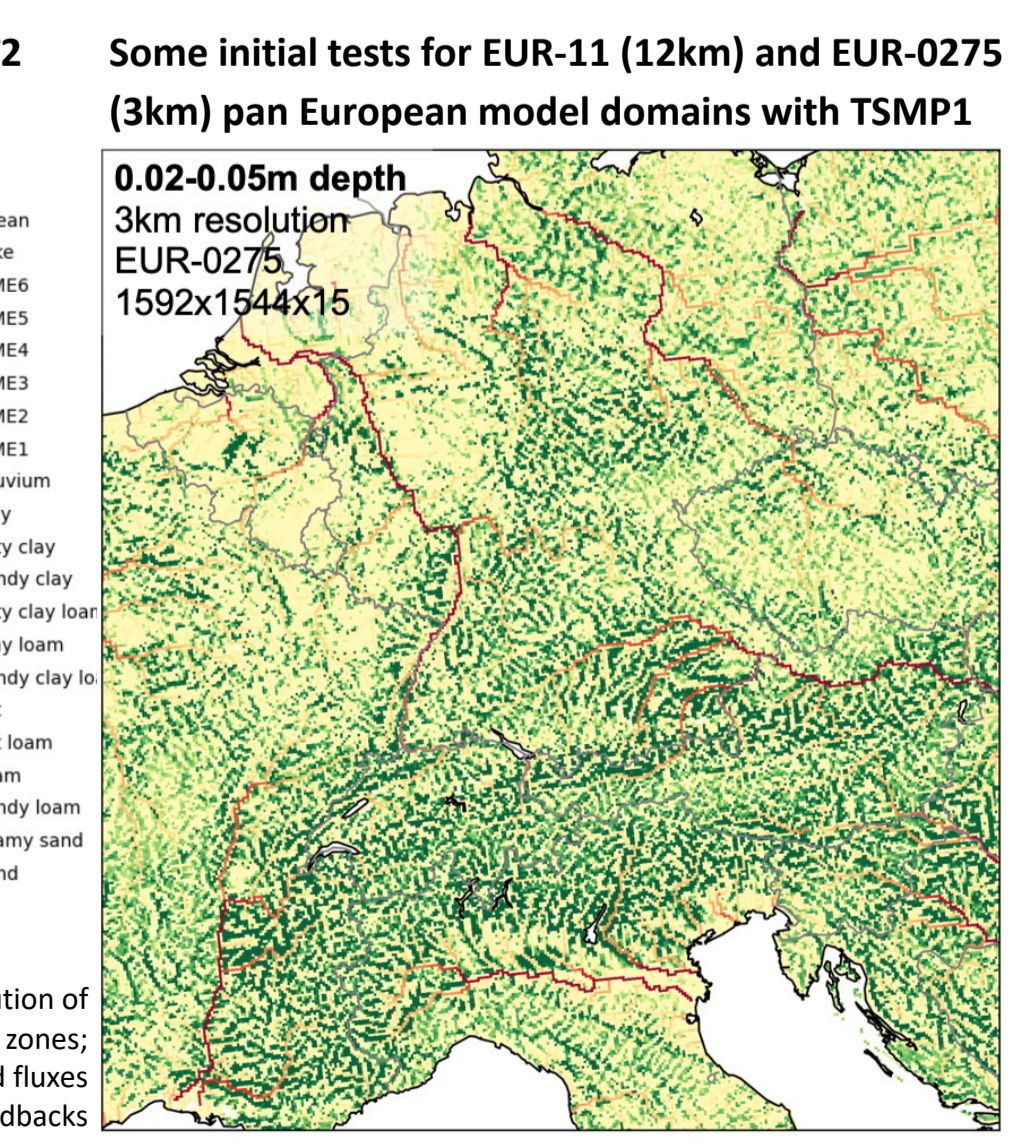
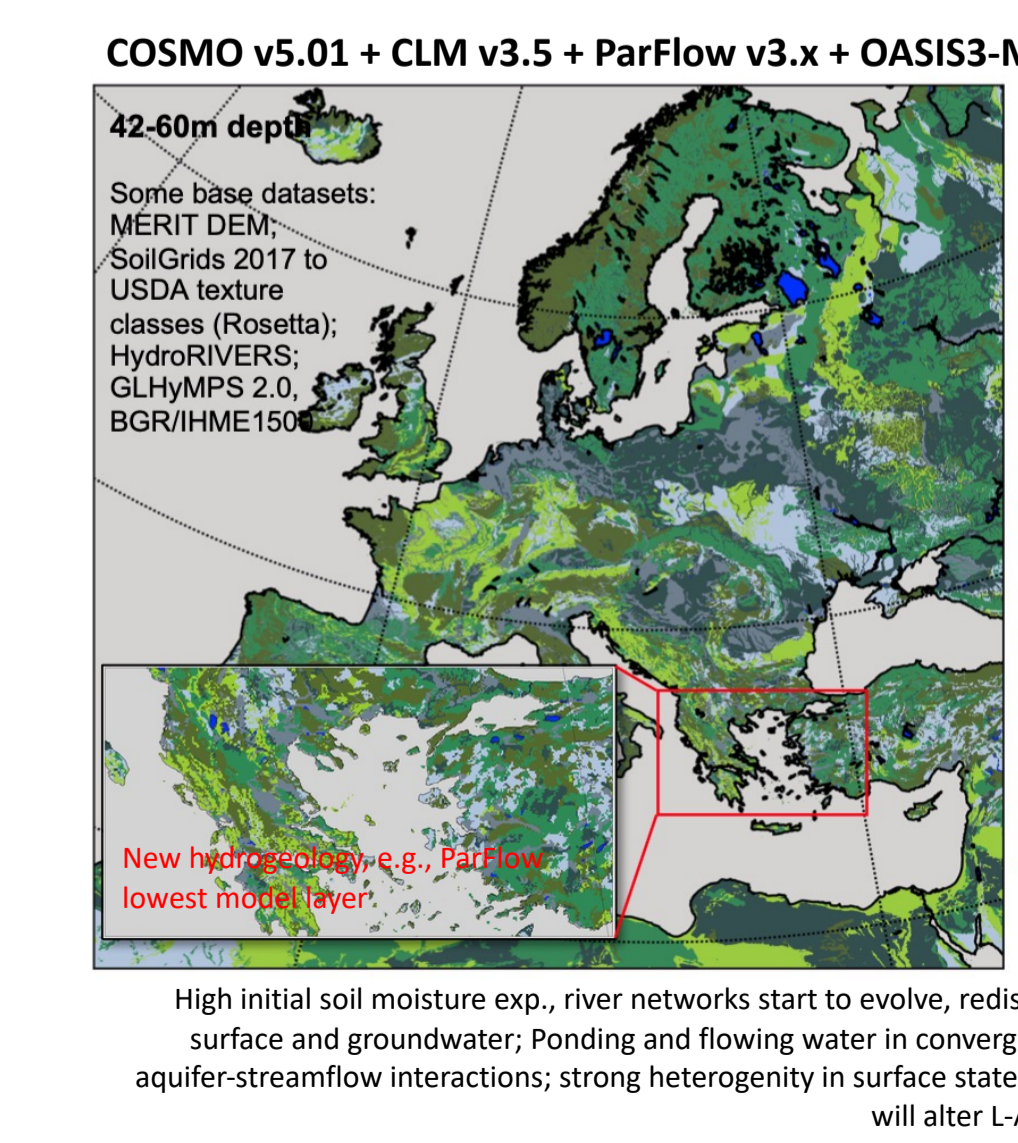
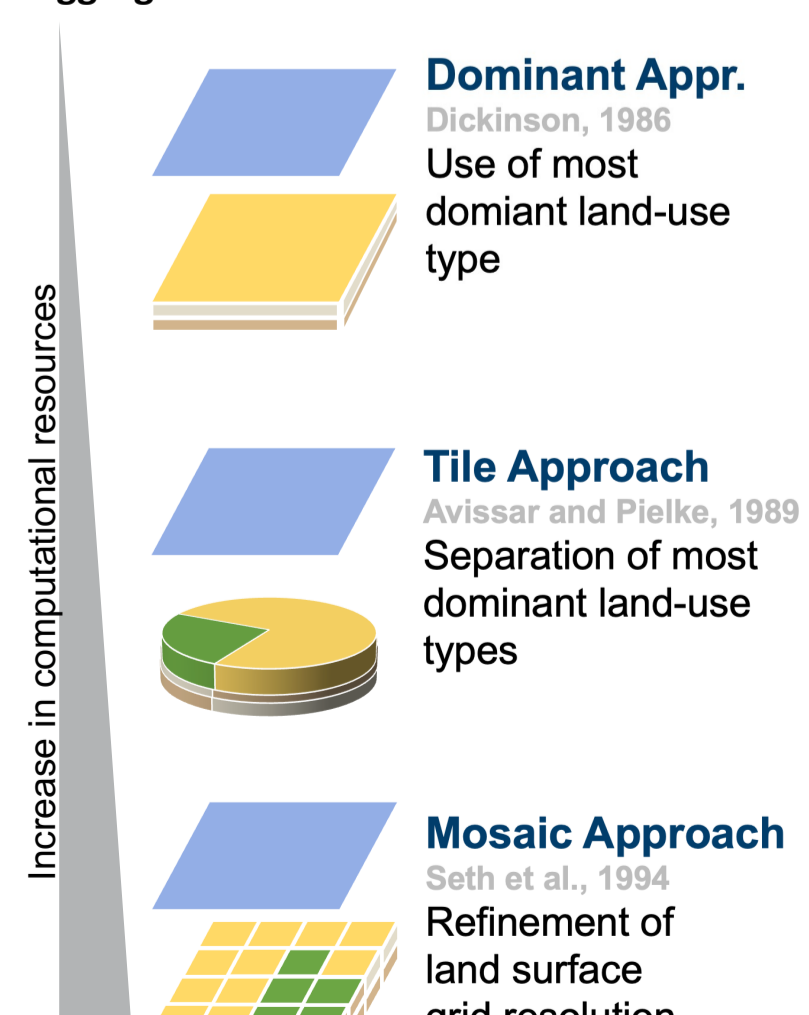
- Preparation of static fields, model configurations, workflow engines, model functionality, code modernisation, test runs, etc. (Wagner, Hartick, Rigor, Poll, Goergen, van Hulten)
- TSMP2 model improvements (ICON radiation treatment, eCLM I/O streams, ParFlow soil-ice scheme, etc.) (Poll, van Hulten, Rigor et al.)
- TSMP-PDAF, DA functionality, additional/modular observational input (CRNS, GRACE); continuous version updates; Python-clone of DA step for testing/method development; new and updated testcases (Keller et al.)



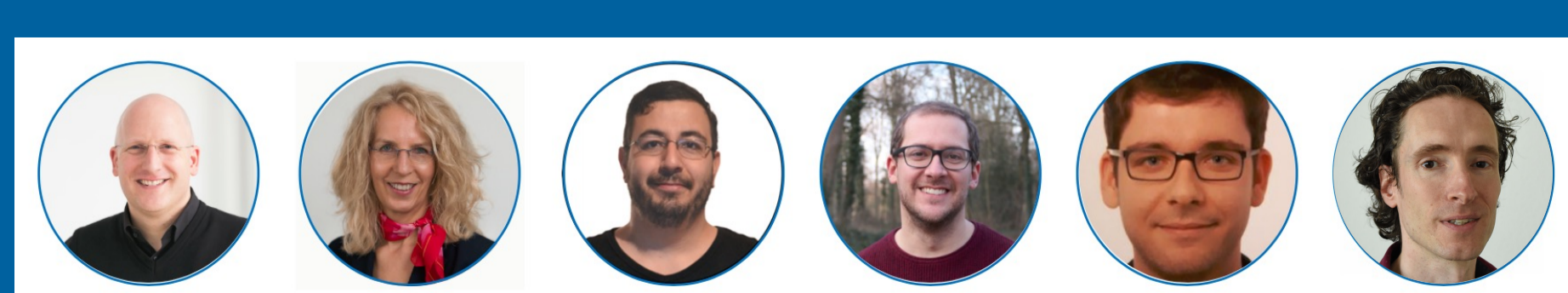
Z04 own research (D02 run participation; CORDEX contribution; surface flux exchange; use modular HPC)

- Added value in coupled (km-scale) pan-European climate-mode frontier simulations (EUR-11, EUR-0275, R13807)
- L-A coupling: 3D vs 1D hydrodynamics in ParFlow, with/without anthropogenic water use, impact of transient aerosols
- Contribution to upcoming new CORDEX-CMIP6 runs with TSMP, towards higher complexity RESMs
- Flux exchange over heterogeneous surfaces
- Implementation and efficient use of latest heterogeneous modular HPC systems (CPU+GPU), with TSMP, ParFlow-GPU offloading

Significant land surface heterogeneity, flux-aggregation methods become relevant



Z04 team from FZJ and UB



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https://gitlab.jsc.fz-juelich.de/detect/detect_z03_z04

