From Catchments as Organised Systems to Models Based on Functional Units

Final Report – phase II subproject E: Towards consistent predictions of water and energy cycles in intermediate scale catchments;

Phase I subproject S: An adaptive process based model framework for water-, energy- and mass cycles in lower mesoscale catchments

1 General Information

1.1 DFG reference number

EH 409/3-1 and ZE 533/12-1

1.2 Applicants

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1.3 Topic

Towards consistent predictions of water and energy cycles in intermediate scale catchments

1.4 Report- and Funding period

01.01.2012 – 31.12.2019

1.5 List of the most relevant publications

a) Peer-reviewed journal articles – first authors

Ehret, U., Gupta, H. V., Sivapalan, M., Weijs, S. V., Schymanski, S. J., Blöschl, G., Gelfan, A. N., Harman, C., Kleidon, A., Bogaard, T. A., Wang, D., Wagener, T., Scherer, U., **Zehe, E.**, Bierkens, M. F. P., Di Baldassarre, G., Parajka, J., van Beek, L. P. H., van Griensven, A., **Westhoff, M. C.**, and Winsemius, H. C.: Advancing catchment hydrology to deal with predictions under change, Hydrol. Earth Syst. Sci., 18, 649–671, https://doi.org/10.5194/hess-18-649-2014, 2014.

Ehret, U., van Pruijssen, R., Bortoli, M., Loritz, R., Azmi, E., and **Zehe, E.**: Adaptive clustering: reducing the computational costs of distributed (hydrological) modelling by exploiting time-variable similarity among model elements, Hydrology and Earth System Sciences, 24, 4389-4411, 10.5194/hess-24-4389-2020, 2020.

Neuper, M., and **Ehret, U.,** Quantitative precipitation estimation with weather radar using a data- and information-based approach, Hydrol. Earth Syst. Sci., 23, 3711-3733, 10.5194/hess-23-3711-2019, 2019.

Westhoff, M. C., and **Zehe, E.**: Maximum entropy production: can it be used to constrain conceptual hydrological models?, Hydrology And Earth System Sciences, 17, 3141-3157, 10.5194/hess-17-3141-2013, 2013.

Westhoff, M. C., **Zehe, E.,** and Schymanski, S. J.: Importance of temporal variability for hydrological predictions based on themaximum entropy production principle, Geophysical Research Letters, 41, 67-73, 10.1002/2013gl058533, 2014.

Westhoff, M., Zehe, E., Archambeau, P., and Dewals, B.: Does the Budyko curve reflect a maximum-power state of hydrological systems? A backward analysis, Hydrology And Earth System Sciences, 20, 479-486, 10.5194/hess-20-479-2016, 2016.

Zehe, E., Ehret, U., Blume, T., Kleidon, A., Scherer, U., and **Westhoff, M.**: A thermodynamic approach to link self-organization, preferential flow and rainfall-runoff behaviour, Hydrology And Earth System Sciences, 17, 4297-4322, 10.5194/hess-17-4297-2013, 2013.

Zehe, E., Ehret, U., Pfister, L., Blume, T., Schroeder, B., **Westhoff, M.**, Jackisch, C., Schymanski, S. J., Weiler, M., Schulz, K., Allroggen, N., Tronicke, J., van Schaik, L., Dietrich, P., Scherer, U., Eccard, J., Wulfmeyer, V., and Kleidon, A.: HESS Opinions: From response units to functional units: a thermodynamic reinterpretation of the HRU concept to link spatial organization and functioning of intermediate scale catchments, Hydrology And Earth System Sciences, 18, 4635-4655, 10.5194/hess-18-4635-2014, 2014.

b) Peer-reviewed journal articles – co-authored

Azmi, E., **Ehret, U.**, Weijs, S. V., Ruddell, B. L., and Perdigão, R. A. P.: Technical note: “Bit by bit”: a practical and general approach for evaluating model computational complexity vs. model performance, Hydrol. Earth Syst. Sci., 25, 1103–1115, https://doi.org/10.5194/hess-25-1103-2021, 2021.

Bauer, H.-S., T. Schwitalla, V. Wulfmeyer, A. Bakhshaii, **U. Ehret, M. Neuper** and O. Caumont (2015): Quantitative precipitation estimation based on high-resolution numerical weather prediction and data assimilation with WRF - a performance test. 2015, 10.3402/tellusa.v67.25047.

Darscheid, P., Guthke, A., and **Ehret, U.**, A maximum-entropy method to estimate discrete distributions from samples ensuring nonzero probabilities, Entropy, 20, 601, 10.3390/e20080601, 2018.

Kleidon, A., **Zehe, E., Ehret, U.,** and Scherer, U.: Thermodynamics, maximum power, and the dynamics of preferential river flow structures at the continental scale, Hydrol. Earth Syst. Sci., 17, 225-251, 2013.

Loritz, R., Hrachowitz, M., **Neuper, M., and Zehe, E**.: The role and value of distributed precipitation data in hydrological models, Hydrology and Earth System Sciences, 25, 147-167, 10.5194/hess-25-147-2021, 2021.

Perdigão, R. A. P., **Ehret, U**., Knuth, K. H., and Wang, J., Debates: Does Information Theory Provide a New Paradigm for Earth Science? Emerging Concepts and Pathways of Information Physics, Water Resources Research, 56, e2019WR025270, 10.1029/2019wr025270, 2020.

Thiesen, S., Darscheid, P., and **Ehret, U**., Identifying rainfall-runoff events in discharge time series: a data-driven method based on information theory, Hydrol. Earth Syst. Sci., 23, 1015-1034, 10.5194/hess-23-1015-2019, 2019.

c) Other Publications

Azmi, E., **U. Ehret,** J. Meyer, R. **van Pruijssen,** A. Streit, and M. Strobl, Clustering as Approximation Method to Optimize Hydrological Simulations, in Euro-Par 2019: Parallel Processing – 25th International Conference on Parallel and Distributed Computing, Göttingen, Germany, August 26–30, 2019, Proceedings. Ed.: R. Yahyapour. Ed.: R. Yahya-pour, edited, pp. 256-269, Springer International Publishing, Cham, 2019.

Prieto, C., **U. Ehret,** and G. Nearing, Using information theory in Earth sciences, Eos, 99, https://doi.org/10.1029/2018EO107389. Published on 10 October 2018, 2018.

2 Final progress report

This report summarizes the outcomes and achievements of CAOS phase II project E. The project was a direct continuation of the phase I projects S ("An adaptive process based model framework for water-, energy- and mass cycles in lower mesoscale catchments") and C ("Quantitative Precipitation Estimation by exploiting the Potential of Advanced Radar Observations and High-resolution Data Assimilation").

2.1 Research questions and objectives

One main objective of phase I project S was to develop an adaptive process-based model for water-, energy-, and mass flows for lower mesoscale catchments using Elementary Functional Units (EFU) as model entities. This idea rests on the overarching CAOS hypothesis that structured patterns of topography, soil, vegetation and biota are co-evolutionary fingerprints of past water, energy, and nutrient flow regimes, which is reflected by the existence of functional units of a distinct hydrological behaviour (Zehe et al., 2014). The other objective was to explore to which extent a thermodynamic perspective and in particular, thermodynamic optimality may advance hydrological modelling and theory (Zehe et al., 2014; Ehret et al., 2014). Phase Project E further advanced distributed modelling of water-, energy- and mass cycles in intermediate scale catchments by addressing the following research questions:

- How to balance necessary complexity and parsimony of hydrological models?
- How to compare models of different complexity in a fair manner and which data/information sources are most important to discriminate the structurally most adequate model?

As an important prerequisite to address these questions, our further objective was to improve and provide quantitative rainfall estimates (QPE) adequate for high-resolution modelling on the lower mesoscale.

Our main hypotheses to address these questions were

- H1: We propose least critical zone entities termed Elementary Functional Units (EFU) as least model entities. EFUs are horizontally homogeneous with respect to the terrestrial properties controlling the gradients and resistances driving land surface –atmosphere energy exchange. This implies they may be treated one dimensionally with respect to vertical water and heat fluxes sustaining the energy balance, in case ergodic conditions are fulfilled.
- H2: The critical zone in the landscape is composed of relatively few, typical, recurring combinations of EFUs that belong to a few typical EFU classes. Landscapes co-evolved into typical, recurring patterns of EFUs along the potential gradients driving lateral water flows during rainfall driven conditions. We name these typical hillslope scale patterns Lead Topologies (LT). Comparable to EFUs and EFU classes, there exist relatively few, typical, recurring types of Lead Topologies, called Lead Topology classes.
- H3: Functional similarity is a scale and context depend emergent property. EFUs (or LTs) of the same class in a similar state and exposed to similar forcing should produce either a similar energy balance or similar stream flow generation by reflecting similar internal dynamics. For models hierarchically built from EFUs and LTs, this implies that such sets of (temporarily) similar EFUs (or LTs), can be grouped to Dynamical Functional Units (DFUs), and their dynamics and responses can with sufficient precision be described by computing the dynamics of just one or a few group representatives and by assigning the results back to all group members.
- H4: Trustworthy distributed rainfall estimates are at least as important as distributed information about the terrestrial system to compile a structurally adequate model at the lower mesoscale. This can be achieved by i) combining multi-sensor precipitation observations from C-band weather radar, vertical radar (MRR), distrometers, and in situ measurements, or by ii) high-resolution weather modeling in combination with high-frequency data assimilation.

2.2 Project developments and conducted research

2.2.1 Thermodynamic optimality as constraint for hydrological model predictions

Within the first funding phase we explored to which extent a thermodynamic perspective may advance and deepen hydrological theory and modelling. Specifically we:

- Tested alternative ways for coupling different process domains and for the executing sequence in hydrological models, by focusing on energy conversion rates associated with hydrological processes.
- Explored whether thermodynamic optimality offers ways for improving model predictions by constraining model parameter sets or even allowing for a-priory uncalibrated predictions.

The first bullet was addressed in phase I project I and phase II project F, which developed and tested a particle based approach for simulating soil water flow in the matrix and in vertical preferential pathways during rainfall driven conditions. (Jackisch and Zehe, 2018). Mass and energy exchange between both domains was successfully characterised with a thermodynamic re-interpretation of the Bernoulli equation as further detailed in the corresponding final report.

Westhoff and Zehe (2013) addressed the second bullet in a Monte Carlo study to explore whether thermodynamic optimality, in fact Maximum Entropy Production MEP, provides a feasible constraint for conceptual model parameters in an HBV type model. They found a small intersect between parameter sets matching the water balance and those that maximized entropy production when a single parameter of the beta store soil moisture accounting scheme. Unfortunately, the intersection was zero when additionally parameters of the sequence of reservoirs controlling runoff concentration were varied. The reason for this is that water flux in HBV-type models are not driven by potential gradients and our efforts to define suitable proxies were not successful. We concluded that MEP is of low use for reducing parameter uncertainty of conceptual models, because these models are not thermodynamically consistent. This is a valuable insight to define the necessary requirements for testing thermodynamic optimality approaches.

Westhoff et al. (2014) investigated furthermore the effect of the frequent assumption of a steady state forcing when searching for thermodynamic optimal model parameters. Starting point was a study of Kleidon and Schymanski (2008), which showed with a simple “electric circuit” model representing the partitioning of rainfall into evaporation and runoff, that one resistance could predicted using MEP when the other one was known. We showed analytically that the previous assumption of a constant forcing leads to an optimum flow resistance that only depends on the known flow resistance of the other flux, but neither on the annual precipitation input nor on gradients driving runoff and evaporation. As this was not in accordance with our perception, we translated the electrical circuit into an equivalent reservoir model where evaporation is driven by a steeper potential gradient than runoff. When driving this model with a periodic stationary forcing representing wet and dry seasons a second maximum in entropy production emerged, that became dominant in case of a long dry seasons. Further analysis showed that the optimum flow resistance and thus the partitioning rainfall into runoff and evaporation depended on the ratio of the gradient driving evaporation and the total rainfall amount. We showed that this ratio corresponds to the dryness index and a plot of the evaporative index against this dryness index resulted in a curve that was highly similar to the Budyko curve. Using an expanded model, Westhoff et al. (2016) showed that the Budyko curve can be derived using the Maximum Power principle as a constraint and that this approach explains offsets of selected water and energy limited MOPEX catchments from the theoretical curve based on the duration of the dry season and the amount of months without evaporation (Fig. 1). In line with this, phase I project D and phase II project C showed that Maximum Power in combination with a specification of the Carnot limit allowed feasible predictions of sensible and latent heat fluxes with astonishingly simple models as detailed in the corresponding final report.

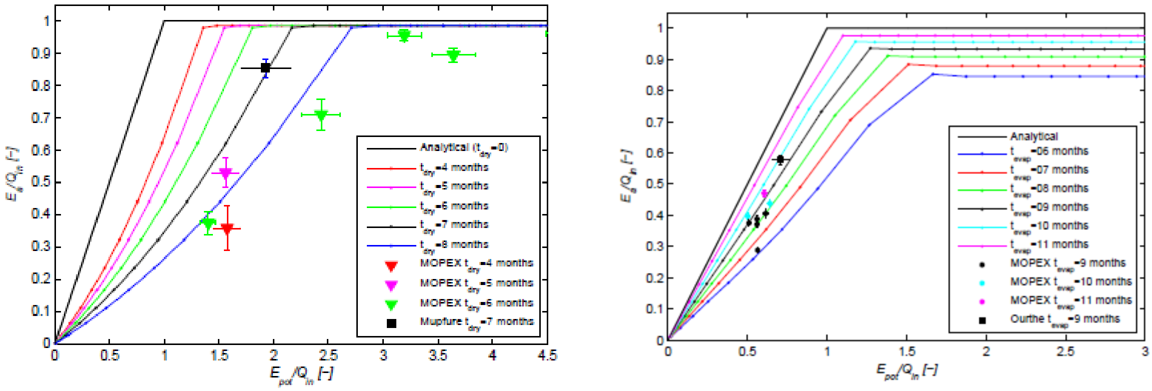

Figure 1: Sensitivity to periodic dry spells in the optimised forward Budyko curve and selected arid MOPEX catchments having at least 1 month with a median rainfall < 2.5mm month^{-1} and a coefficient of variance < 0.5 for all months with a median rainfall > 25mm month^{-1} (a). Sensitivity to "on and offset in actual evaporation" in the forward model and energy limited MOPEX having a coefficient of variance < 0.12 for monthly median rainfall and with at least 1 month with a median maximum air temperature < 0°C. A month is considered to have no actual evaporation if the monthly median maximum air temperature < 0°C. Error bars indicate 1 standard deviation are determined with bootstrap sampling. Source Westhoff et al. (2016).

Furthermore, we jointly developed a thermodynamic framework to quantify conversion and dissipation of free energy associated with rainfall runoff (Zehe et al. 2013). Rainfall runoff processes are associated with conversions and dissipation of capillary binding energy (in fact chemical energy), potential energy and kinetic energy. Although being very small compared to the land surface energy balance, these energy fluxes are the key to explain portioning of rainfall into runoff components and storage dynamics form an energy centred point of view and they provide a common framework for explaining why preferential flow phenomena occur. Preferential flow path leads to faster fluid flows, because they reduce dissipative losses due to an increased hydraulic radius in the rill or river network compared to sheet to overland flow in surface water systems (Berkowitz and Zehe, 2020). Subsurface preferential flow of water reduces dissipative losses as well, because friction occurs mainly at macropore or fracture walls, while frictional interactions in the matrix occur along the entire inner surface. Reduced dissipation and faster fluid flow imply a more energy efficient throughput of water, mass and chemical species through the entire system (in case of flow paths spanning the entire system).

While this increased energy efficiency is, at first sight, a purely diagnostic observation, it explains the growth phase of rill and river networks, and why they grow in a self-reinforcing and directed fashion. This is because flow against the gradient implies higher stream power, defined as volumetric flow times the geopotential gradient, which means that more kinetic energy can be transferred to the sediments (Kleidon et al., 2013). The related higher erosion rates imply an upstream growth of river networks. A faster flow against the driving gradient means that the latter becomes depleted more rapidly, which in turn means that entropy is produced. This slow negative feedback works against structural growth of river network and this implies the existence of a metastable maximum power state as shown in Kleidon et al. 2013).

In Zehe et al. (2013) we related the total soil water potential to its free energy, and analyzed free energy changes associated with overland flow and soil water dynamics within a physically based model study using the Weiherbach data set. By varying the density of preferential flow paths in soil from zero up to a density where surface runoff vanished completely, we found two optima that maximized the energy dissipation averaged across all recharge events. One of these optima allowed an acceptable prediction of the rainfall runoff response of the Weiherbach without any calibration to discharge data (Fig. 2).

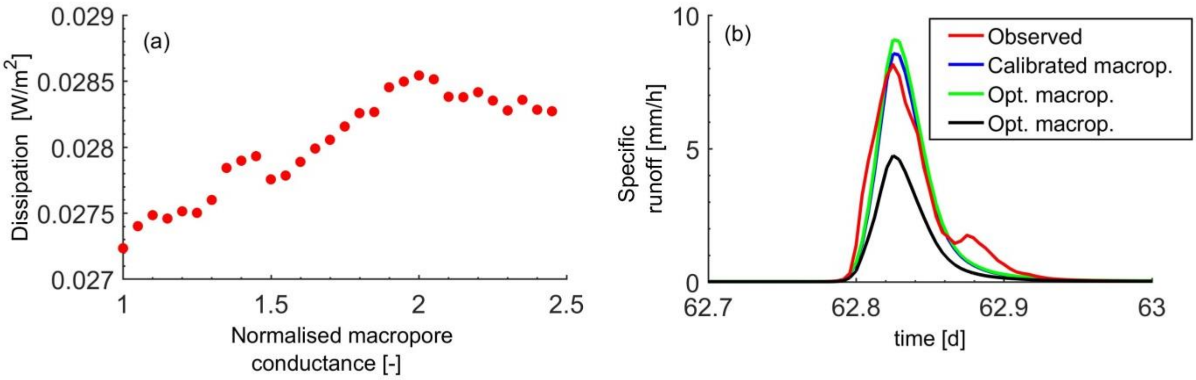

Figure 2: Total dissipation of free energy of soil water as function of the normalised macropore conductance. The latter is total hydraulic conductivity summed of all macropores in the model domain divided to the saturated hydraulic conductivity of the soil matrix. (b) Simulated specific runoff with a macroporosity calibrated to match discharge response of the catchment (Calibrated macrop.), uncalibrated simulations based on the two local optima macroporosities (Opt. macrop.) and observed specific discharge at the catchment outlet (source Zehe et al., 2013, adapted).

As one of the optima performed well with respect to predict rainfall runoff, we concluded that the catchment is in an optimal structure as well. The “open point” in the argumentation is that earthworms cannot directly benefit from the enlarged power in soil water fluxes. Zehe et al. (2013) postulated furthermore the existence of two distinct thermodynamic regimes of rainfall runoff behavior. Cohesive soils work predominantly in the C-regime as free energy dynamics of soil water is dominated by changes in its capillary binding energy; while grained soils in steep terrain work in the P-regime as potential energy dominates energy conversions in soil. Phase II project F further explored these ideas by expanding the thermodynamic framework of rainfall runoff generation as detailed in the corresponding final report.

2.2.2 The CAOS model – an adaptive model for the water and energy balance of lower mesoscale catchments

Phase I project S started with the development of a process-based model for water-, energy-, and mass flows for lower mesoscale catchments using elementary functional units (EFUs) as building blocks. Key emphasis was on an explicit representation of connective flow structures such as macropores, pipes, or rills. Scope of this development was to create model framework, which allows testing of the central CAOS hypotheses, i.e. feasibility of an adaptive grouping of EFUs into cluster of similar functioning and to represent those by a single of few representatives thereby avoid redundant simulations. The idea of the dynamic adaptive modelling was to reduce computational loads such that the model becomes applicable in engineering practice without too much compromising the physics governing unsaturated zone (preferential) flow process. In phase I a first version of the CAOS model was implemented in Matlab in a fully object oriented manner. Here we put major emphasis on the physical soundness of governing equations, the explicit treatment of vertical and lateral preferential flow in connected networks and a technically sound and efficient numerical solution of the model equations (Zehe et al., 2014). Despite of the physical soundness and the computational efficiency of this CAOS version, the object structure did not allow quantification of information flows associated the simulated hydrological dynamics. As the latter greatly facilitates the quantification of similarity of model objects (see previous section) and the implementation of a dynamic adaptive grouping (see next section), phase II project E started a complete new development of a second CAOS model version. This effort put much more emphasis on a sufficiently flexible object structure and the possibility to track mass, information and energy fluxes in the model.

We have developed a fully object-oriented model designed to represent water-related processes in the atmospheric boundary layer, the soil surface, unsaturated and saturated zone and vegetation. The model is coded in Matlab with full versioning control in GitHub. In this framework, we have so far implemented all but the boundary layer and vegetation processes; these are still represented by observations. As outlined in the work program, the model represents 3d processes by multi-1d representations to reduce computational efforts and explicitly represents all stocks and fluxes of mass (surface water flow, matrix and preferential vertical infiltration, subsurface lateral flow in preferential flow structures, saturated flow in alluvial floodplain, river flow) and energy (thermal energy, geopotential energy, capillary energy, kinetic energy). All structural and state variables in the model are physical quantities, i.e. they can be directly estimated from observables. The main model structure and elements are shown in Fig. 3 and have been chosen to match hypotheses H1 and H2. A model-setup exists for the entire Attert basin, which was used to generate high-resolution (5 min, few m²) model runs for several sub basins. We also developed an advanced GIS- and Matlab-based preprocessing tool for model setup in new catchments.

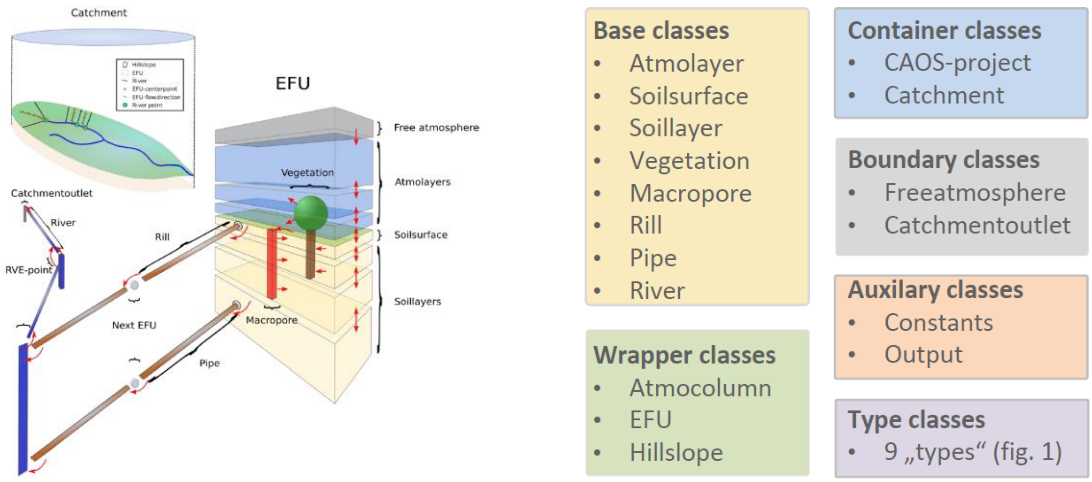

Figure 3: Left panel: CAOS model structure. Right panel: CAOS model classes

While the model as it meets all the desiderata formulated in the project outline, it is far from being complete: The current version misses essential process representations related to the boundary layer and soil-atmosphere exchange as well as processes related to evapotranspiration. The reason for these misses is mainly that we underestimated the challenges of formulating all processes in the model with a full representation of all related stocks and fluxes of mass and energy and under the constraint of the Maximum Power optimality principle. We are still convinced of this approach and will continue to work on it, but are somewhat sobered about the related efforts. We also faced considerable computational difficulties (high computation times and numerical error), which we found to be mainly due to the high model resolution and the simple numerical scheme (explicit forward-in-time). We are convinced that these issues can be overcome by dynamical clustering, a new method for avoiding redundant computations we developed in this project and which we explain in section 2.4. Through dynamical clustering, we can maintain high spatial resolution, a requirement for physically meaningful parameterization, increase the model time-stepping to reduce numerical error and still keep computational efforts at an acceptable level.

We must thus admit that we so far clearly didn't live up to our goal to deliver a model of intermediate and adaptive complexity that allows feasible simulations of the water and energy balance of lower mesoscale catchments. Despite to this drawback the efforts were valuable as they stimulated a fruitful exchange with other teams of the CAOS research unit. The feasibility of adaptive modelling was nevertheless successfully tested using two essentially different model structures: a simple conceptual hydrological model SHM (Ehret et al., 2020) and the physically based model CATLFLOW Loritz et al., 2020) as detailed below.

2.2.3 Information-based multiscale verification

One of the main challenges of working in an interdisciplinary research group is to handle the large variety of data not only from the point of view of storage and exchange, but also in terms of finding a common framework in which the value of these data can be evaluated. We found information theory, due to its generality, to be extraordinarily well suited for this task. In information theory, the value of data can, irrespective of its units and disciplinary origin, be expressed as information content, which can also be interpreted as uncertainty reduction. Adding to these advantages, (algorithmic) information theory offers ways to express the information content of both data and models in a single quantity, bit, which is also the fundamental unit when processing data or running models on computers, nowadays the main tool of science. We found information theory applied to the problems of hydrology in general and to those of our research group in particular (e.g. Neuper and Ehret, 2019; Thiesen et al., 2019; Darscheid et al., 2018) to be an extremely powerful tool. It opened a whole new perspective of looking at data and models, allowed direct comparison of the usefulness of all sorts of data and all sorts of models, from data- to physics-based, and allows through the concept of entropy a natural linkage to thermodynamics and thermodynamic optimality (Perdigao et al., 2020), one of the core topics in CAOS. This was clearly more than we expected and we consider this together with adaptive modelling (section 2.2.5) as the main contribution of our project to the research group. Fig. 4 gives a flavour of information theories' generality, showing a generalized way of model evaluation (Azmi et al., 2020). We would also like to emphasize that our CAOS-induced interest in information theory has given rise to a series of conference sessions, summer schools and workshops (Prieto et al., 2018). For CAOS, we have used information concepts to evaluate the information content of data (section 2.5), for model comparison (Fig. 2, right panel), to analyse structural and functional similarity and as a basis for dynamical clustering (section 2.4).

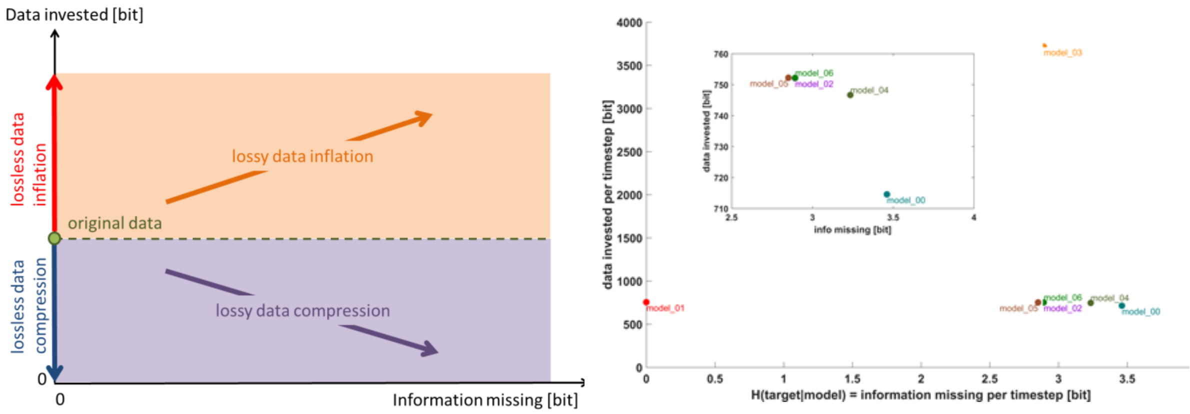

Figure 4: Left panel: Generalized evaluation of models in terms of efficiency (data invested) and effectiveness (information missing). Right panel: Model efficiency vs. model effectiveness for six hydrological models differing in terms of model structure, resolution, and numerical scheme.

2.2.4 Comparing competing model structures on the lower mesoscale

The goal of this work package was to set up and compare various hydrological models (CATFLOW, CAOS, ROGER and NOAH-MP) to evaluate which of them makes best use of available data and which best copes with the challenges of simulating lower mesoscale hydrological system dynamics. The CAOS model was set up for the entire Attert basin, but simulations so far only exist for selected sub-basins (see section 2.1). Due to time constraints, neither ROGER nor NOAH-MP were set up, but we set up the process-based, high-resolution CATFLOW model (see also report of project F) and the conceptual model LARSIM, which was made available to us by the operational water service in Luxembourg. We also compiled a comprehensive 6-year quality-checked data set sufficient to set up and run most hydrological models in the Attert basin (structural data: digital elevation model, land use, geology, soils, river network; forcing and validation data: precipitation, air temperature, global radiation, wind, relative humidity, discharge; data are from both CAOS and operational services). CATFLOW was used extensively to evaluate hydrological similarity (see report of project F). We also designed and coded a new conceptual model called SHM (Simple Hydrological Model, see Fig. 5) and applied it to the Attert basin. We designed it mainly as a testbed for dynamical clustering (see section 2.2.5), but it is also available for model comparison.

As our framework for model evaluation turned out to be much more generally applicable than envisaged (see section 2.2), we decided to shift from the original set of models to a more diverse range encompassing purely data-based and conceptual models. Our main insight was that with just a few well-chosen predictors (mainly precipitation sums and gauge observations of the immediate past), purely data-based models perform as good as conceptual models. While this is somewhat disenchanting for conceptual hydrological modellers, it demonstrates how much information about discharge is contained in both the meteorological drivers and in the memory of the system.

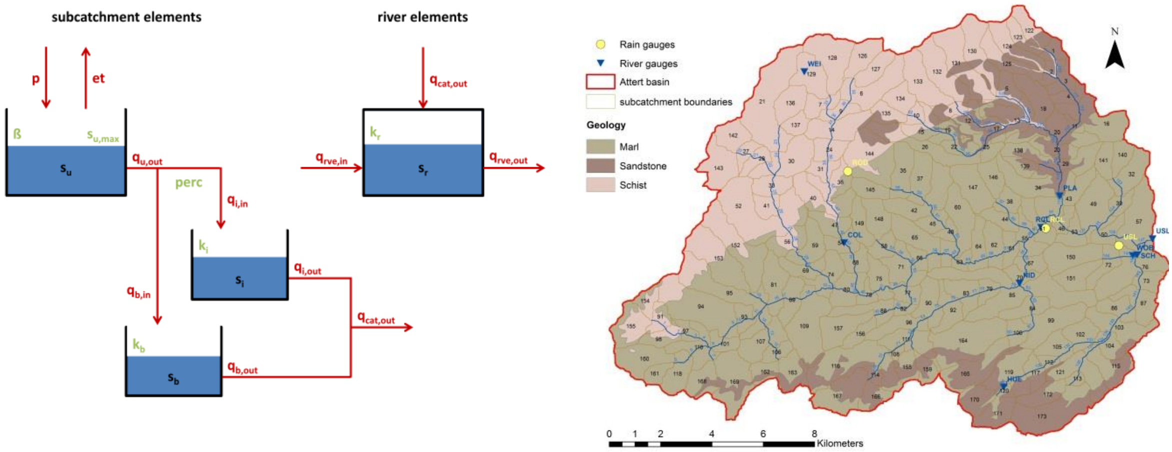

Figure 5: Left panel: Structural elements, parameters, state variables and fluxes of the SHM model. Right panel: Attert basin with gauges and SHM sub catchment and river elements.

2.2.5 Adaptive model clustering: improving modelling efficiency by using of dynamic functional similarity

One of the main goals of CAOS was to find and analyse space-time patterns of structural and functional similarity in lower mesoscale catchments, to identify their dominant controls and to find ways to capitalize on them e.g. for interpolation, design of monitoring networks, and adaptive modelling. The main goal of adaptive modelling is to reduce computational efforts of distributed and high-resolution modelling to facilitate application at larger scales or for longer periods of time. The main idea is to avoid redundant computations by clustering similar model elements, and then to infer the dynamics of all elements in a cluster from just a few representatives. For adaptive clustering to make sense, three preconditions must be fulfilled: Existence of i) many model elements of ii) the 'same kind', with potentially similar behaviour but iii) only weak interaction. These preconditions are largely fulfilled for sub catchments or hillslopes in distributed hydrological models. They occur in large numbers, there is only little or no interaction among them as they act in parallel, connecting to rivers, and as the critical zone in the landscape is composed of relatively few, typical, recurring combinations of its constituents there is potential for similarity among model elements which we can exploit. Along these lines Ehret et al. (2020) developed ways to analyse dynamical similarity of model elements and re-cluster them during run time using concepts from information theory. Expressing (diss-)similarity by information entropy revealed striking patterns of spatial redundancy and seasonal and event-specific variation (see Fig. 6).

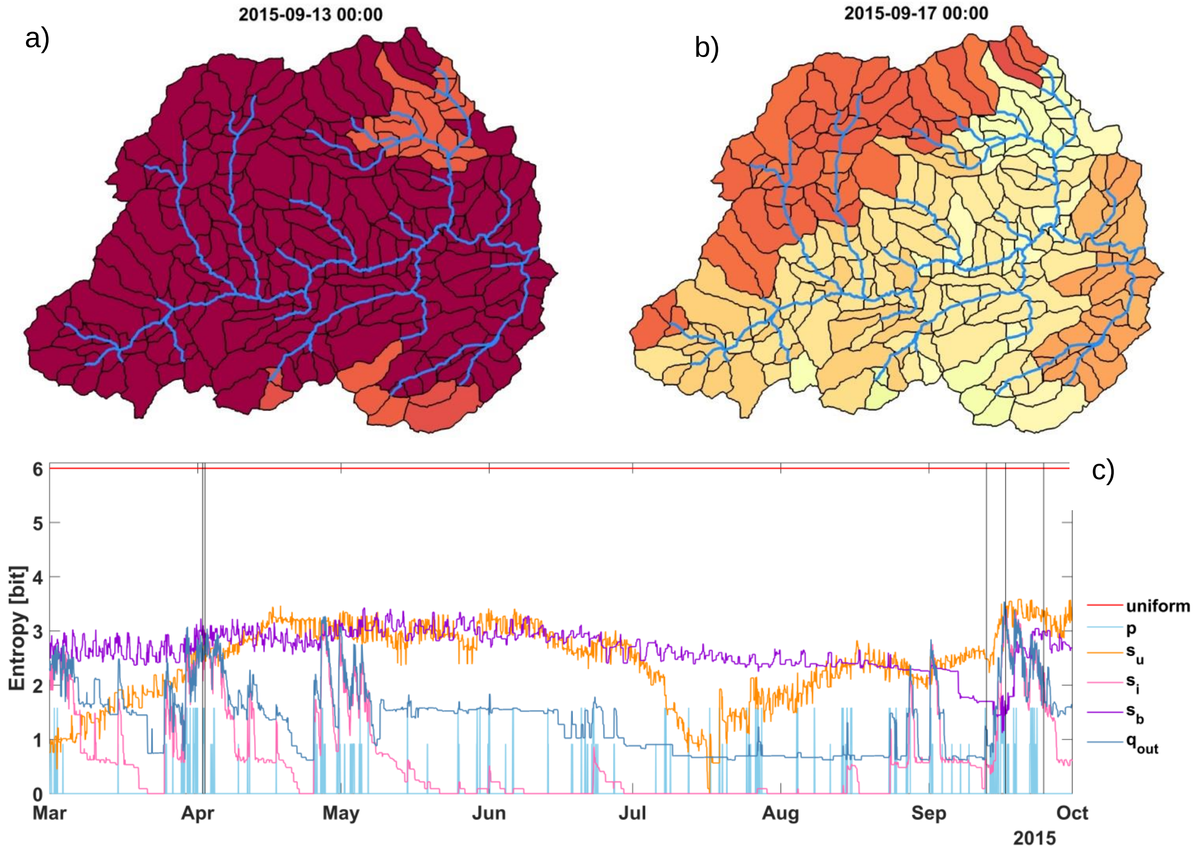

Figure 6: Spatial pattern of SHM Attert sub catchment outflow for two times. After a long dry spell, almost all sub catchments show the same low outflow (ab). After spatially distributed rainfall, a mixed pattern controlled by geology and spatial rainfall distribution appears (b, compare also Fig. 2 a). Time series of Entropy of forcing (p = precipitation), states (su = unsaturated zone storage, si = interflow reservoir storage, sb = base flow reservoir storage) and fluxes (qout = sub catchment outflow) of all 173 sub catchments in the SHM Attert model (c).

One of the key findings in this context was that prior knowledge of these patterns can greatly reduce computation times of spatially distributed models while the related decrease of simulation quality is in most cases acceptable. For the SHM (Ehret et al., 2020) we obtained N execution acceleration by a factor of four at acceptable model simulation qualities (see Fig. 7).

Along similar lines but with emphasis on the role of spatially gridded precipitation for runoff simulations, Loritz et al. (2021) explored the feasibility of adaptive modelling using a set of 42 hillslopes in CATFLOW. These were structurally identical to a representative hillslope model of the Colpach (Loritz et al. 2017) and driven by the gridded, radar based precipitation field. This study revealed that distributed precipitation did generally clearly improve stream flow simulations compared to simulations with spatially uniform precipitation, particularly during the summer season, where frequently localised convective events occur. For two selected rainfall runoff events Loritz et al. (2021) showed that adaptive modelling is also feasible for so called physically based models (Fig. 8). This is explained by the dissipative nature of runoff generation, which implies that memory of the system on distributed forcings and systems states is rather short. This makes hydrological systems distinctly different from the atmosphere. Azmi et al. (2019) further explored the potential of adaptive clustering with a focus on computational efficiency.

Dynamical clustering holds a great potential to maintain high-resolution, processed-based modelling at the lower mesoscale and at larger scales, while still keeping a lid on execution times. We consider this together with the discovery of information theory as a framework for learning and prediction as our main contribution to the goals of the CAOS project. They will be in the focus of our future research activities.

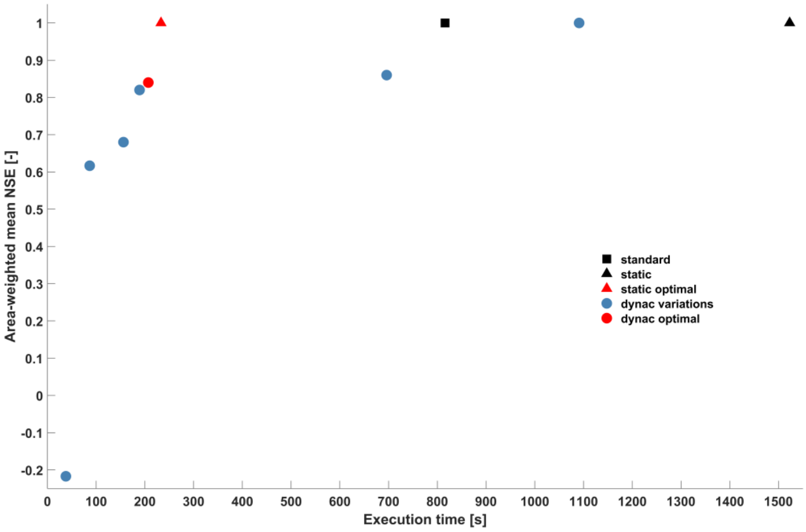

Figure 7: Evaluating variations of the SHM Attert model in terms of efficiency expressed by execution time, and effectiveness expressed by Nash-Sutcliffe efficiency (compare Fig. 2). Compared to a standard full resolution run ('standard'), static optimal clustering based on prior analysis ('static optimal'), and dynamical clustering done during model execution ('dynac variations', 'dynac optimal') greatly reduces execution time while NSE deteriorates only to a lesser degree.

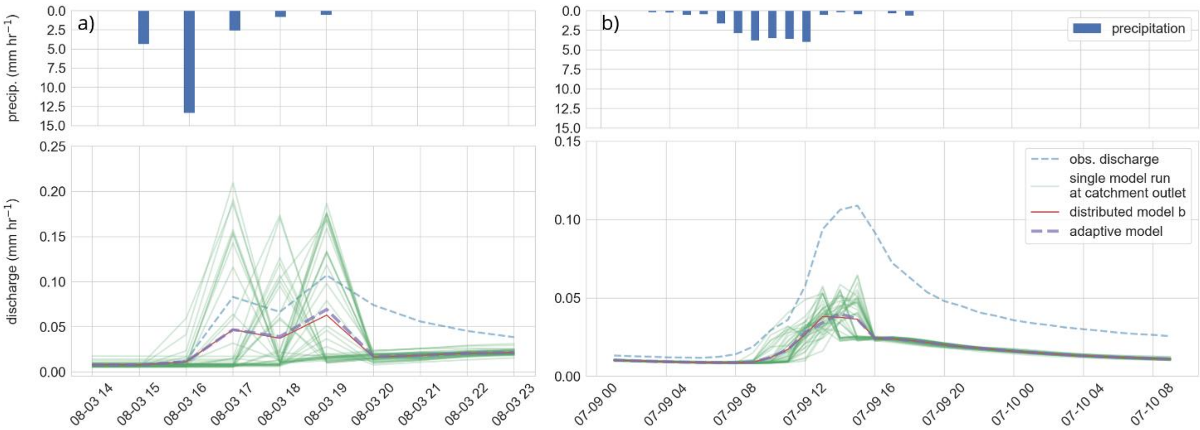

Figure 8: a) rainfall-runoff event I and b) rainfall-runoff event II. Blue bars in the upper panel show the average precipitation of the precipitation field for each time step (mm hr-1). The green curves in the lower panel represent a single gridded model of the distributed model b; red line the area-weighted mean of the distributed model; purple dashed line the area-weighted mean of the adaptive model and dashed blue line the observed specific discharge of the Colpach.

2.2.6 Adequate precipitation input for high-resolution hydrological modelling on the lower mesoscale

High-resolution and high-quality quantitative precipitation estimation (QPE) is one of the key prerequisites for hydrological modelling on the lower mesoscale; improving QPE was therefore part of both CAOS phases. During phase I, our focus was on i) installing and operating a sensor network consisting of two micro rain radar, six distrometers and several rain gauges, ii) setting up of the WRF-NOAH-MP modelling and data assimilation system, with a resolution of 1 km encompassing the Attert catchment, for model-based QPE, and iii) verification of both model- and observation-based QPE methods (Bauer et al., 2015). In Fig. 9, spatial rainfall estimates by kriging-based station interpolation, radar, WRF-based QPE using data assimilation in rapid update cycles, and a merger of radar- and WRF-based QPE are shown for the passage of frontal rain in the morning of Sep 26, 2012. All QPE methods capture the front-like shape of the rainfall field. However, if we take the radar image (upper right panel) as the 'truth', the WRF QPE field is too small and underestimates rainfall. The merging field preserves the overall structure and extent of the radar rainfall field, but rainfall magnitudes resemble that of the station interpolation field, at least in the vicinity of stations (where the kriging variance is small).

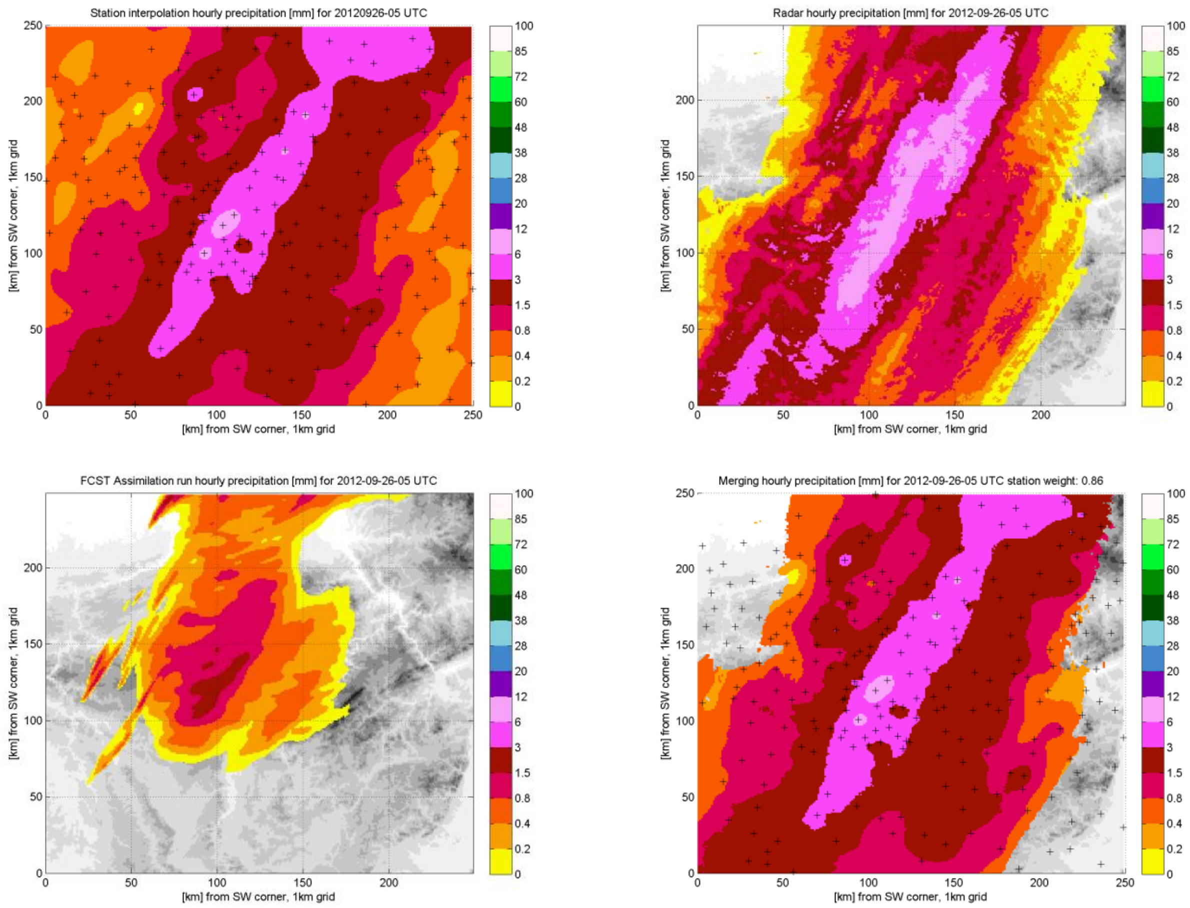

Figure 9: Spatial rainfall estimates for the verification domain (Luxemburg-centered) for Sep. 26, 2012, 04-05:00 UTC. Upper left: Station interpolation, upper right: data from C-band radar Wideumont, lower left: WRF rapid update cycle assimilation run, lower right: merging of station and radar data.

During phase II, our attention shifted away from model-based QPE. This is a miss, as we promised to do so in the project outline, and it is mainly due to two reasons: First, the phase I results of merging observation-based QPE and WRF simulations did not show a clear advantage over observation-based QPE alone, and second the related WRF modelling efforts were quite substantial. In phase II, the main focus of the Hohenheim group operating WRF was on local, very-high resolution modelling of distinct events (see report of project C), which absorbed most of their capacities. As a consequence, we focused on multi-sensor observation-based QPE in phase II, while still remaining in close contact with the Hohenheim group. As we maintained our monitoring network of rain gauges, distrometers, vertical radars and weather radars throughout both phases of CAOS, we now have a very comprehensive dataset to offer to the hydro-meteorological community. We used this data set to quantify the value of various observables for estimating ground precipitation (Neuper and Ehret, 2019). Applying the language of information theory as described in section 2.2, we were able to quantify the information content of data and the effect of sample size in the same unit, bit, and evaluated these results against benchmark maximum entropy estimates. As can be seen in Fig. 10, a careful choice of predictors is essential for robust QPE, as increasing the number of predictors quickly demands very large learning data sets. Also, ground observations proved to be the most informative predictor for distances up to 8 km, beyond quality-checked weather radar data were better.

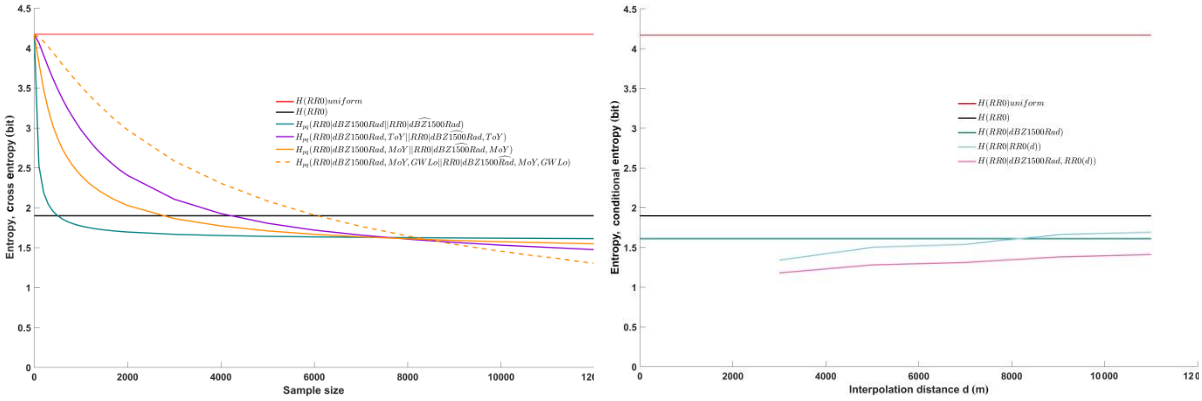

Figure 10: Left panel: Entropy of ground rainfall for no predictors available (black line), entropy of the benchmark maximum entropy uniform distribution (red line), cross entropies between conditional distributions of the target given one, two and three predictors for the full data set and samples thereof (green, purple, yellow and dashed yellow lines, respectively). The “^” symbol indicates a sample. Right panel: Entropy of ground rainfall for no predictors available (black line, same as in left panel); entropy of the benchmark uniform distribution (red line, same as in left panel); conditional entropy of the target given reflectivity as predictor (green line); conditional entropy of the target given station rain rate observations as a function of interpolation distance (light blue line); and conditional entropy of the target given reflectivity and rain rate at stations as a predictor as a function of interpolation distance (pink line).

2.3 Qualification of young researchers

Martijn Westhoff conducted CAOS research as Post-Doctoral scientist during phase I project S. During this period, he prepaired a successful Marie Curie proposal and was afterwards appointed as assistant professor of hydrology at the Free University of Amsterdam. Stefanie Thiesen completed her PhD-theses within project E. Moreover, the project provided food for five MSc theses.

2018/02: PhD project Stephanie Thiesen: A data- and information-based approach to hydrological learning and prediction (ongoing).

2017/07: PhD project Rik van Pruijssen: Hydrological modeling of mesoscale catchments (ongoing).

2015/05: PhD project Malte Neuper: Quantitative Niederschlagsschätzung mit Hilfe eines Regenradars: Multiparametraler Ansatz für mesoskalige Einzugsgebiete mit Fokus auf Variabilität und Anpassung der Tropfengrößenverteilung (ongoing).

2019/11: MSc project Marina Bortoli: Analyzing hydrological similarity to reduce redundancies in distributed hydrological model by dynamical clustering (ongoing).

2019/01: MSc project Katharina Teltscher: Using information theory for data-based modeling of flood predictions. A case study for the river Regen, Bavaria.

2018/01: MSc project Gyöngyver Vargane Ujfalussy: Comparative analysis of conceptual and data-based hydrological models in the Attert catchment, Luxembourg.

2017/06: MSc project Paul Darscheid: Quantitative analysis of information flow in hydrological modelling using Shannon information measures.

2016/09: MSc project Rik van Pruijssen: Modeling infiltration and soil water dynamics within the CAOS framework: a partitioned matrix flow approach.

Moreover, we organized six conferences, summer and winter schools and three sessions at international conferences related to CAOS research topics.

In line with the DFG guidelines we omitted explicit listing of invited talks (6) and contributions to international workshops and conferences (11) related to the CAOS project.

3 Summary

The combination of hydrological process research with concepts drawing from thermodynamics and information theory turned out to be most helpful for defining functional similarity and linking this to structural properties and spatial organisation of the landscape. Hydrological processes are on a very general level dissipative, as storage, mixing and release of water as runoff and latent heat are generally associated with conversions, dissipation and export of free energy. The thermodynamic perspective is hence the natural choice to understand the interplay of the mass and free energy balance of hydrological systems, explain their dependence on the prevailing forcing, landscape structure and state. While fluxes of mass, energy, momentum or entropy are driven by potential gradients (e.g. in temperature and hydraulic head), it is the flow resistance in the control volume that determines how much energy the fluid dissipates when flowing through the soil, macropore, river net, tree or aquifer. Key emphasis of our experimental design was hence on the characterisation of those landscape characteristics and state variables, which control gradient and resistances, with a strong emphasis on preferential pathways. The energy perspective is also helpful to explain the ubiquitous preferential flow phenomena. Preferential flow in connected networks implies a more energy efficient throughput of water and matter through the system. This because they reduce flow-weighted dissipative losses due to an increased hydraulic radius in the rill or river network compared to sheet overland flow (Kleidon et al., 2013) or in subsurface connected preferential pathways compared to matrix flow (Zehe et al., 2013). At the end of the day, water prefers the path of minimum resistance, due to the highly dissipative nature of porous media and shallow overland flow. The tradeoff between energy dissipation via overland flow or via preferential infiltration, implies also the existence of an optimum soil infiltration capacity maximizing total energy dissipation. While we do not claim this to be a universal constrain on rainfall splitting into overland flow and infiltration, it provides at least a testable hypothesis for uncalibrated predictions (Zehe et al., 2013). In phase II, we combined the thermodynamic approach with an information perspective. Information theory is ideal to provide a common framework to evaluate the value of data, because it can, irrespective of its units and disciplinary origin, be expressed as information content, which can also be interpreted as uncertainty reduction. Information theory applied an extremely powerful tool, for instance to identify rainfall runoff events (Thiesen et al. 2019), designing a general framework for model evaluation and exploring the feasibility of hydrological models with adaptive complexity (Ehret et al., 2020). Information theory is well suited for diagnosing the degree of redundancy in a distributed model setup of 19.4 km^2 large Colpach catchment consisting of 105 different hillslopes (Loritz et al. (2018). In this study entropy was used as measure for diversity and thus uncertainty of the simulated runoff of the hillslope ensemble at each time step. Although the entropy of the ensemble was rather dynamic in time, it never reached the maximum value. The latter implies that hillslopes contribute in a unique fashion to streamflow, while a zero entropy means that all hillslope yield an indistinguishable runoff response. Functional similarity is, as stated in our central hypothesis, nothing static but a dynamic attribute, which jointly reflects changing spatial organization of processes in the landscape and their dissipative nature. Information entropy is hence well suited to diagnose the degree of organization of a system state or a process based on its deviation from the entropy maximum, because its definition is equivalent to Gibb's definition of physical entropy in statistical mechanics. We thus conclude that uncertainty about and organization of a system state are two sides of the same medal related.

With respect to our main hypotheses, we have relied on H1 when designing the CAOS model, and the models' acceptable performance is a (weak) proof. However, we found ample evidence of H2 and H3 when investigating ways for adaptive modelling. With respect to H4, we have made substantial progress in non-parametric, multi-sensor QPE but could not add to the phase I insights about QPE based on weather modelling and data assimilation.