RoGeR v3.0.~~3~~4 – a process-based hydrological toolbox model in Python

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Abstract. Although water availability and water quality are equally important for an effective water resources management, to date, a combined representation of soil water balance components and water quality components in Python ~~is~~are not available. The new RoGeR toolbox contains models that can be used for the quantification of hydrological processes, fluxes and stores, but also solute transport processes based on StorAge selection. This study

10 presents the code structure and functionalities of RoGeR developed as a scientific model toolbox following defined open-source software guidelines. RoGeR uses five different computational back-ends covering just-in-time compilation, parallelism and graphical-processing units that might be used for optimizing computational performance. We show that graphical-processing unit computing ~~have~~has the greatest potential to improve computation time and energy usage, especially for large modelling experiments. A simple modelling experiment highlights the capabilities

15 of the new RoGeR model toolbox. We simulated the soil water balance, stable water isotope (^{18}O) transport and corresponding travel time distributions ~~through~~of the ~~soil of a grassland plot~~Eberbaechle catchment, Germany, for a three-year period. ~~Further development of RoGeR as a scientific software is possible and also needed~~ Due to the current limitations for a variety of process components ~~and~~further development of RoGeR as a scientific software is needed. Future modifications are easily possible due to the open software architecture of RoGeR.

1 Introduction

The interplay between the water and solute mass balance (e.g. oxygen-18, chloride or nitrate) and its related flow and transport in the soil-vegetation-atmosphere interface plays an important role for the understanding of hydrologic systems (e.g. Benettin et al., 2017). However, measurements ~~for~~of their states and fluxes are neither in space nor in time ubiquitously available (Beven, 2011). Thus, soil hydrological models, soil-vegetation-atmosphere-transfer

25 (SVAT) models and distributed catchment models are indispensable tools to complement measurements (e.g. for a better process understanding) and to make predictions (e.g. future climate impacts, land cover changes or in ungauged catchments). Currently, there are many models in hydrology and the landscape of models is highly diverse (from simple conceptual models to complex physically-based models). One reason for this large and diverse landscape of models is that hydrologist still disagree about modelling concepts (Weiler and Beven, 2015). Despite the large number

30 of models, however, there is a lack of reproducibility in computational hydrology (Hutton et al., 2016; Reinecke et al., 2022). The main reasons for this lack of reproducibility are poorly documented codes and workflows (e.g. Reinecke et al., 2022,), code being too complex (e.g. Reinecke et al., 2022,), unavailable code (e.g. Reinecke et al., 2022being not availability and), missing input data (e.g. Reinecke et al., 2022not available ().), a lack of calibration standards and a lack of standards dealing with uncertainties.

35 Simulating the hydrological processes at the soil-vegetation-atmosphere interface including solute mass balance and transport with a high spatial and/or temporal resolution still requires long computation time. Thus, For reasons of computational performance, hydrological models such as HYDRUS (Šimůnek et al., 2016), Daisy (Abrahamsen and Hansen, 2000), HYPE (Lindström et al., 2010), EcH2O-iso (Kuppel et al., 2018) or mHM (Heße et al., 2017; Kumar et al., 2020; Kumar et al., 2013; Samaniego et al., 2010) are written in low-level programming languages such as

40 Fortran or C++. However, these languages are hard to read, to learn and are usually not included in the curriculum of hydrology-related degree programs. By contrast, high-level programming languages are easier to read and to learn, but computation takes about 3-5 times longer than equivalent code in low-level programming languages (Häfner et al., 2021). Therefore, high-level programming languages have the potential to foster reproducibility. Recently, high-level open-source programming languages such as R or Python gained popularity in the hydrological modelling

45 community. Especially Python is currently the most popular programming language among software users (e.g. IEEE Spectrum, 2022; PYPL, 2022; Stack Overflow, 2021). Hydrological models quantifying the hydrological cycle that are written in Python, for example, are SUPERFLEX (Dal Molin et al., 2021; Fenicia et al., 2011), CWatM (Burek et al., 2020) and UniFHy (Hallouin et al., 2022) but none of these models consider transport of solutes, and they generally focus at the catchment scale. To date, only rsas (Harman, 2015) implemented a solute transport model

50 written in Python. However, rsas does not quantify the water balance and requires hydrological fluxes as input.
For reasons of longer computation times, high-level programming languages are often avoided in spatially distributed hydrological models. One solution to reduce computation time in high-level programming languages is using a just-in-time compiler (JIT). However, Python does not contain a built-in JIT. Instead, Python requires program libraries such as Numba (Lam et al., 2022) or JAX (Bradbury et al., 2018). However, Numba and JAX provide the opportunity

55 to run the code on graphical processing units (GPUs) to decrease computation times. Veros (Häfner et al., 2018; Häfner et al., 2021), an ocean model written in Python using JAX for acceleration, demonstrated that GPU computations are a competitive alternative to central processing units (CPUs). In addition to that, Häfner et al. (2021) could show that GPU computations savessave energy.
The first model version of RoGeR had a focus on the event-based runoff generation (Steinbrich et al., 2021). Therafter,

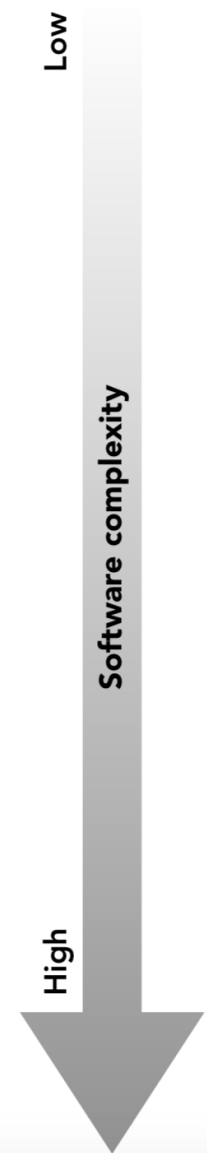
60 RoGeR hadhas been further developed and by adding a routing scheme, surface runoff and subsurface runoff contributions to flooding events could be explicitly simulated (Steinbrich et al., 2021). Additionally, by considering snow hydrological processes, urban hydrological processes and redistribution processes such as evapotranspiration enabled the estimation of the long-term water balance (Steinbrich et al., 2021). Based on the previous development

efforts of the RoGeR model by Weiler (2005), Steinbrich et al. (2016) and Steinbrich et al. (2021), we reimplemented the process-based hydrological model RoGeR in a modular software architecture (e.g. different hydrological processes are implemented in separate modules that can be independently modified) written in Python. Since RoGeR had no implementation for solute transport so far, we include solute transport based on StorAge selection (SAS) functions (e.g. Benettin et al., 2017). We choose a high-level programming language and a modular software paradigm to foster reproducibility and wide-range application in teaching and research. In particular, we aim to facilitate general code understanding, writing new code and debugging code which usually takes most of the time within software projects. To overcome limitations on computational performance, we include the program library JAX.

In the following, we describe the implementation of the new model developed as a scientific software following open-source guidelines. Thereafter, we provide a brief overview about the representation of the hydrological processes and the related solute transport. We further profile the computational performance and energy usage. Finally, we demonstrate the capabilities of the model by simulating a three-year period for a synthetic site.

2 Implementation

2.1 RoGeR as a scientific open-source software

For the development of RoGeR as scientific open-source software, we followed the guidelines presented in Table 1. We defined these guidelines based on van Gompel et al. (2016) and Hall et al. (2022), and on reviewing earth science related software written in Python (e.g. Bakker et al., 2016; Bartos, 2020; Burek et al., 2020; Collenteur et al., 2019; Dal Molin et al., 2021; Häfner et al., 2018; Hallouin et al., 2022; Helmus and Collis, 2016; Kratzert et al., 2022; Mälicke, 2022; May et al., 2022; Rose, 2018; Schwemmle et al., 2021). We suggest that different software concepts might be applied depending on the software complexity. Moreover, including these guidelines in the curriculum of hydrology-related degree programs may lay the foundation for a reproducible future in computational hydrology.

2.1.1 Software architecture

The basic modular structure of the software is adapted from Häfner et al. (2018). The core modules implement hydrological processes and solute transport. As such, these modules represent a toolbox which can be used to build pre-defined models (e.g. a SVAT model by considering only vertical processes). We already provided some pre-defined models, but in general new models can be easily assembled and combined to the level of complexity that is required. Moreover, further processes might be added by writing new modules. In addition to that, further modules are available for the pre-/post-processing, writing the model output and handling computational back-ends. RoGeR is pure Python, hence not all computational bottlenecks might be solvable. In such cases, we recommend writing extensions using Cython instead of using a low-level language which would require a compiler.

2.1.2 Computational back-ends

95 The computations are handled by five different back-ends which are implemented through a function decorator (Häfner et al., 2018). Users have to choose a suitable backend beforehand. The choice depends on programming skills, size of the

Table 1 Guidelines for scientific open-source software in computational hydrology

	Term/Concept	Description	Advantage
Low	Comments	Write meaningful and clear comments within the source code	Comprehensive and reusable source code
	Public access	Store the source code in an online-repository and use version control to enable collaborative development	Transparent and accessible
	License	Regulates usage of the software	Reusable
Software complexity	Versioning	Assigns a new version number after each release (i.e. update of the source code)	Traceable
	Software environment	Use a virtual environment to avoid software conflicts and provide information about software dependencies	Quick installation
	Logger	Captures errors, warnings and progress of computation	Facilitates debugging
	Hands-on-tutorials	Guidance on the application of the software for real case examples	Learnable and lower entry bar for new users
	Online documentation	Contains essential information for installing, using the software and theoretical background (e.g. equations)	Learnable and understandable
	Unit tests	Tests basic functionality of the software	Facilitates maintenance
High	Continuous integration	Runs unit tests on different operating systems and different software stack	
	Profiling	Measures computation time (e.g. of individual modules) or memory usage (e.g. GPU memory)	Supports efficient allocation of computational resources

100 modelling experiment and available computational resources. In the following, we briefly describe the back-ends and give recommendations on the usage:

- numpy: This back-end uses NumPy () for computation and, hence, is easy to use. However, the interpreted execution of the code and running computations on a single CPU may cause performance limitations. We recommend this back-end to beginners and for small-scale modelling experiments. As long as the modelling

105 experiment fits in the memory, there are no specific requirements for the computational resources.

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(left margin label: Software complexity, arrow pointing from Low to High)

- numpy: This back-end uses NumPy (Harris et al., 2020) for computation and, hence, is easy to use. However, the interpreted execution of the code and running computations on a single CPU may cause performance

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       as the modelling experiment fits in the memory, there are no specific requirements for the computational
       resources.

       -    numpy-mpi: The numpy-mpi back-end parallelizes the numpy back-end via mpi4py (Dalcin et al., 2011).
            The size of the modelling experiment might be limited by available memory and number of CPU cores. We
115   recommend this back-end to users with experience in parallelized computations.

       -    jax: The jax back-end is the same as numpy, but code is JIT compiled via JAX (Bradbury et al., 2018). Since
            JAX transforms NumPy code, it is required that all code is NumPy compatible. The JIT compilation leads
            to decreasing computation time (see Sect. 3).

       -    jax-mpi: Same as numpy-mpi, but code is JIT compiled via mpi4jax (Häfner and Vicentini, 2021). This leads
120   to computational speedup (see Sect. 3).

       -    jax-gpu: The code is JIT compiled and computations are performed on GPU which leads to computational
            speedup (see Sect. 3). The jax-gpu backend requires an appropriate GPU. The size of the modelling
            experiment is limited to available to GPU memory. We recommend this back-end to users with advanced
            programming skills.

125   **2.1.3 Discretization and data handling**

      For RoGeR-1D (i.e. no lateral transfer between grid cells), space can be represented either through grid cells or
      polygons. By contrast, RoGeR-2D models (i.e. lateral transfer between grid cells) require a regular grid as spatial
      representation. In order to generate physically meaningful results, we recommend a spatial resolution between 0.25
      m^2 and 25 m^2.

130   RoGeR requires input data for the following variables:
      RoGeR requires input data for the following variables:

           -    precipitation up to 10 minutes time steps
           -    air temperature at daily time steps
           -    potential evapotranspiration at daily time steps
135   -   solute concentrations at daily time steps (only if solute transport is simulated)
                at up to 10 minutes time steps
                air temperature at daily time steps
                potential evapotranspiration at daily time steps
                solute concentrations at daily time steps (only if solute transport is simulated)

140   The 10 minutes time step is required for the detailed representation of the runoff generation processes (i.e. infiltration,
      surface runoff and lateral subsurface runoff). Averaging the input flux for longer time steps leads to an overestimation
      of infiltration and underestimation of overland flow and preferential flow. Hourly precipitation or daily precipitation

datasets can be used with the model and resampled to 10 minutes, however, losing the required temporal variability to correctly simulate the runoff generation processes. For heavy rainfall intensities (the default threshold is > 5 mm/10 minutes), the time step is adapted to 10 minutes (Figure 1). For non-heavy rainfall intensities (<5 mm/10 minutes and > 0 mm/10 minutes), the simulations use an hourly time-stepping. While no rainfall occurs, a daily time step is used. If precipitation data is available with coarser temporal resolution, for example, hourly or daily resolution, we recommend to resample the precipitation data to the required 10 minutes resolution. Depending on the resolution of the available precipitation data, different resampling methods can be applied. For example, hourly date can be linearly interpolated 10 minutes or daily data can be disaggregated (e.g. Förster et al., 2016; Koutsoyiannis and Onof, 2001~~The input data can be either provided as NetCDF files (.nc) or text files (.txt). If input data is provided as~~).

The input data can be a time series or spatio-temporal data (i.e. time series for each grid cell) which is either provided as text files (.txt) or NetCDF files (.nc). If the input data is provided as a time series using text files, the data is internally converted to NetCDF.

Metadata (e.g. units, description) for all variables and constants are defined in single modules as dictionaries (Häfner et al., 2018). From these dictionaries, metadata (e.g. units) is automatically added to the model output data. All model output is written to NetCDF files. A major advantage of the NetCDF format is that I-O operations enables parallel writing with compression (Häfner et al., 2018). This reduces time of I-O operations and the size of output files.

~~For 1D models (i.e. no lateral transfer), space can be represented either through grid cells or polygons. By contrast, 2D models (i.e. lateral transfer between grid cells) require a regular grid as spatial representation. In order to generate physically meaningful results, we recommend a spatial resolution between 0.25 m² and 25 m².~~

2.2 Hydrological model

Different hydrological processes are implemented as modules. In the following, we list the already implemented processes and refer to the module and declare whether the module is tested or testing is still ongoing:

- Surface water storage (*surface.py*; testing is complete)
- Soil water storage (*soil.py*; testing is complete)
- Root zone water storage (*root_zone.py*; testing is complete)
- Subsoil water storage (*subsoil.py*; testing is complete)
- Groundwater water storage (*groundwater.py*; testing is ongoing)
- Transpiration (*evapotranspiration.py*; testing is complete)
- Soil evaporation (*evapotranspiration.py*; testing is complete)
- Interception (*interception.py*; testing is complete)
- Snow accumulation/Snow melt (*snow.py*; testing is complete)
- Infiltration driven by capillary forces (*infiltration.py*; testing is complete)
- Infiltration driven by gravitational forces (*film_flow.py*; testing is ongoing)

- Surface runoff (*surface_runoff.py*; testing is ongoing)

- Lateral subsurface runoff (*subsurface_runoff.py*; testing is ongoing)

- Lateral groundwater flow (*groundwater_flow.py*; testing is ongoing)

- Percolation (sub*surface_runoff.py*; testing is complete)

180 - Capillary rise (*capillary_rise.py*; testing is complete)

- ~~Solute transport and water ages (*transport.py* and *sas.py*; testing is complete)~~

- Crop phenology (*crop.py*; testing is ongoing)

- ~~Nitrogen cycle (*nitrate.py*; testing is ongoing)~~

The main reason for using a modular structure ~~enables,~~ is to support the readability of the code. Another motivation

185 for using a modular structure is to represent a certain process by multiple process formulations that provide different

complexities (Knoben et al., 2019). As such the processes can be combined in multiple ways to build different model

structures. Thus, depending on the chosen process complexity, model structures represent the considered by different

degrees of

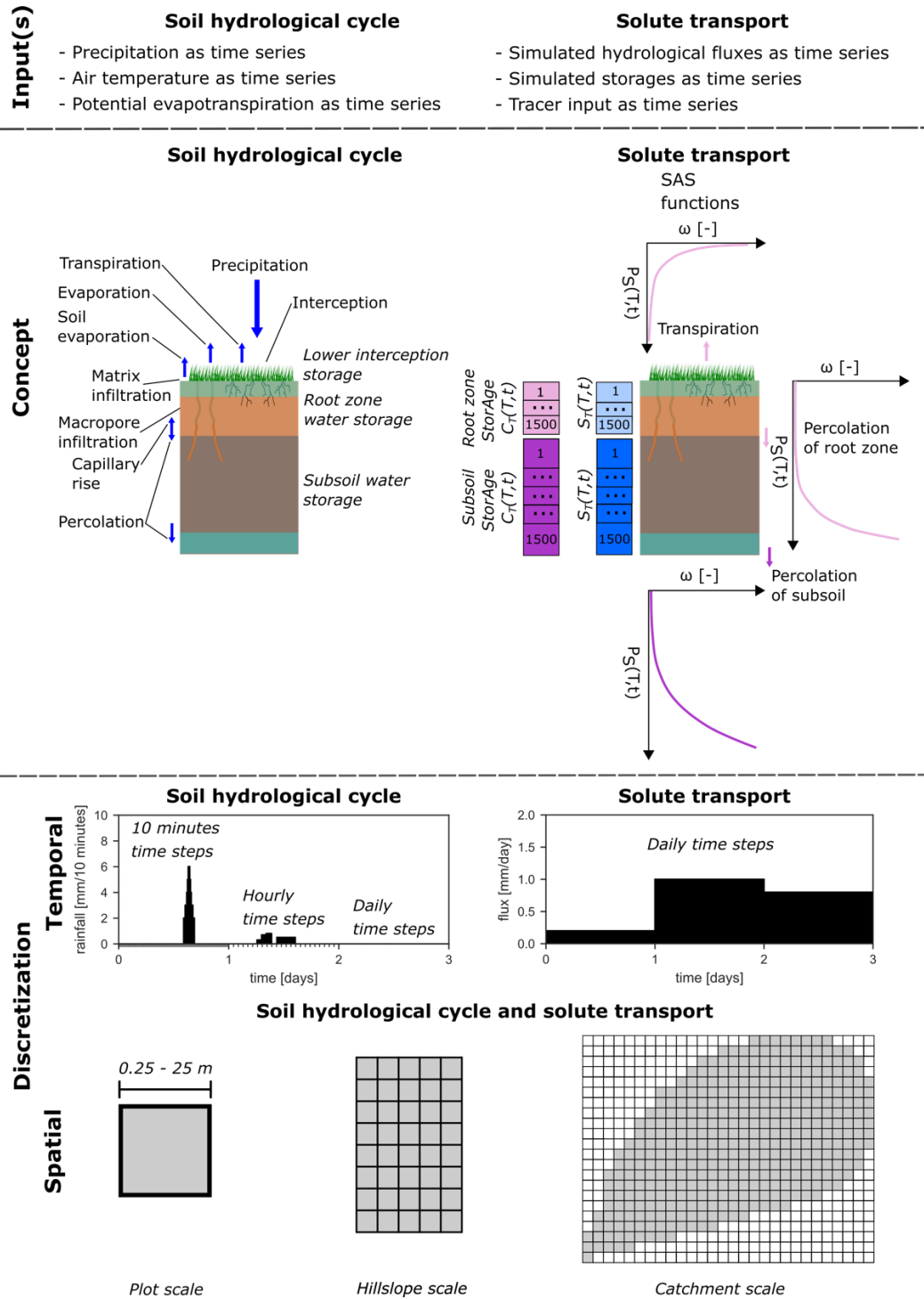



Figure 1 Overview of model inputs, conceptual implementation shown for a single grid cell or unit (Water storages are represented in italic), and temporal discretization of the soil hydrologic cycle and solute transport. Spatial discretization for different scales is the same for the soil hydrologic cycle and solute transport.

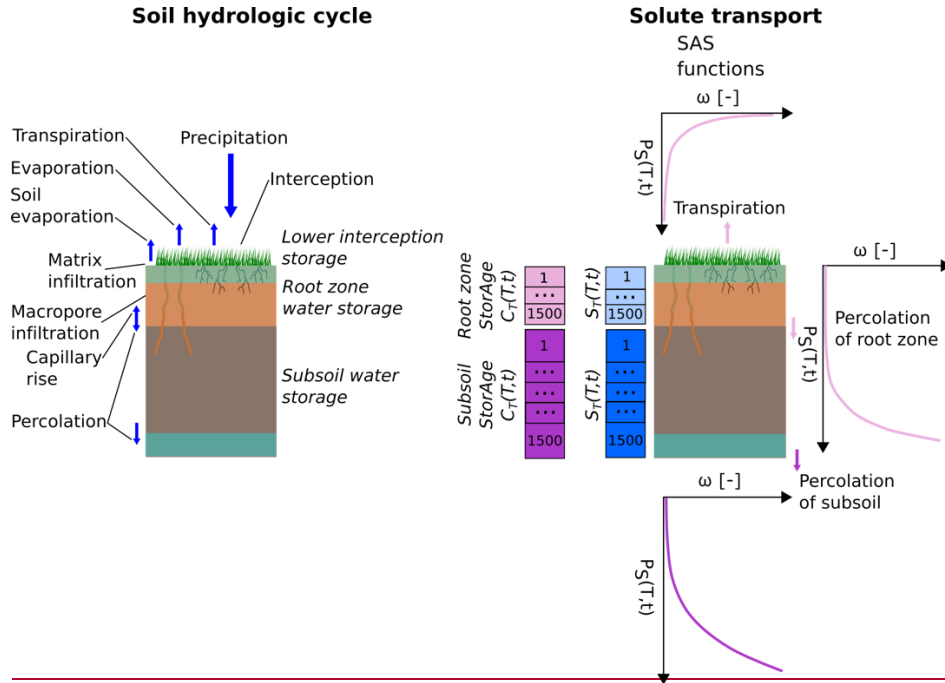
complexity. However, building process-consistent model structures from many different process formulations can be challenging to model users. RoGeR uses single process formulations that constrains the flexibility of the structural

195   complexity. However, we provide pre-defined model structures (i.e. a combination of various hydrological processes and thus building) to ensure a certain model structureprocess consistency. The most basic model structure is shown in Figure 1 and is the basis for more complex model structures. We pre-defined further model structures by adding further hydrological processes (e.g. lateral subsurface flow, crop phenology). For more details about the pre-defined model structures, we refer to the online documentation of RoGeR (Schwemmle, 2023).

200   RoGeR provides representations for bucket-type interception, degree-day based snow accumulation and snow melt (LARSIM-Entwicklergemeinschaft, 2021), soil matrix, macropore and shrinkage crack infiltration (Steinbrich et al., 2016; Weiler, 2005), soil evaporation (Or et al., 2013), vegetation phenology and vegetation-specific transpiration (Steduto et al., 2009), capillary rise from a groundwater table and percolation to the groundwater (Salvucci, 1993) and lateral subsurface runoff (Steinbrich et al., 2016; Stoll and Weiler, 2010). For detailed information (e.g. model

205   equations), we refer to the online documentation of RoGeR (Schwemmle, 2023).

RoGeR solves explicitly the soil water balance (i.e. fluxes update the state in a specific sequence) using an adaptive time-stepping scheme (see Figure 1). The adaptive time stepping provides a better compromise between accuracy and performance compared to fixed time stepping schemes (Clark and Kavetski, 2010). Numerical errors may compensate for model structural errors, we have not evaluated the effect of other time stepping schemes on the numerical errors

210   of RoGeR. Although numerical errors affect the simulations, parameter uncertainty (e.g. Wagener and Gupta, 2005) or input data uncertainty (e.g. Yatheendradas et al., 2008

215   ) may have a stronger impact on the simulations.

2.3 Solute transport model

Solute transport is implemented by a travel-time based approach. Particularly, we use StorAge selection (SAS) functions (Rinaldo et al., 2015). SAS is implemented by specific distribution functions. We assign a distribution function to each hydrological process (Figure 1). Here, we introduce two distribution functions which can be used for

220   SAS and are implemented in the toolbox. The first distribution function is based on a power law and requires only a single parameter k_Q (Fig. 2a). The power law distribution function is given as:

$$\omega_Q(T,t) = k_Q{}^{k_Q} \cdot P_s(T,t)^{(k_Q-1)}$$

(1)

with

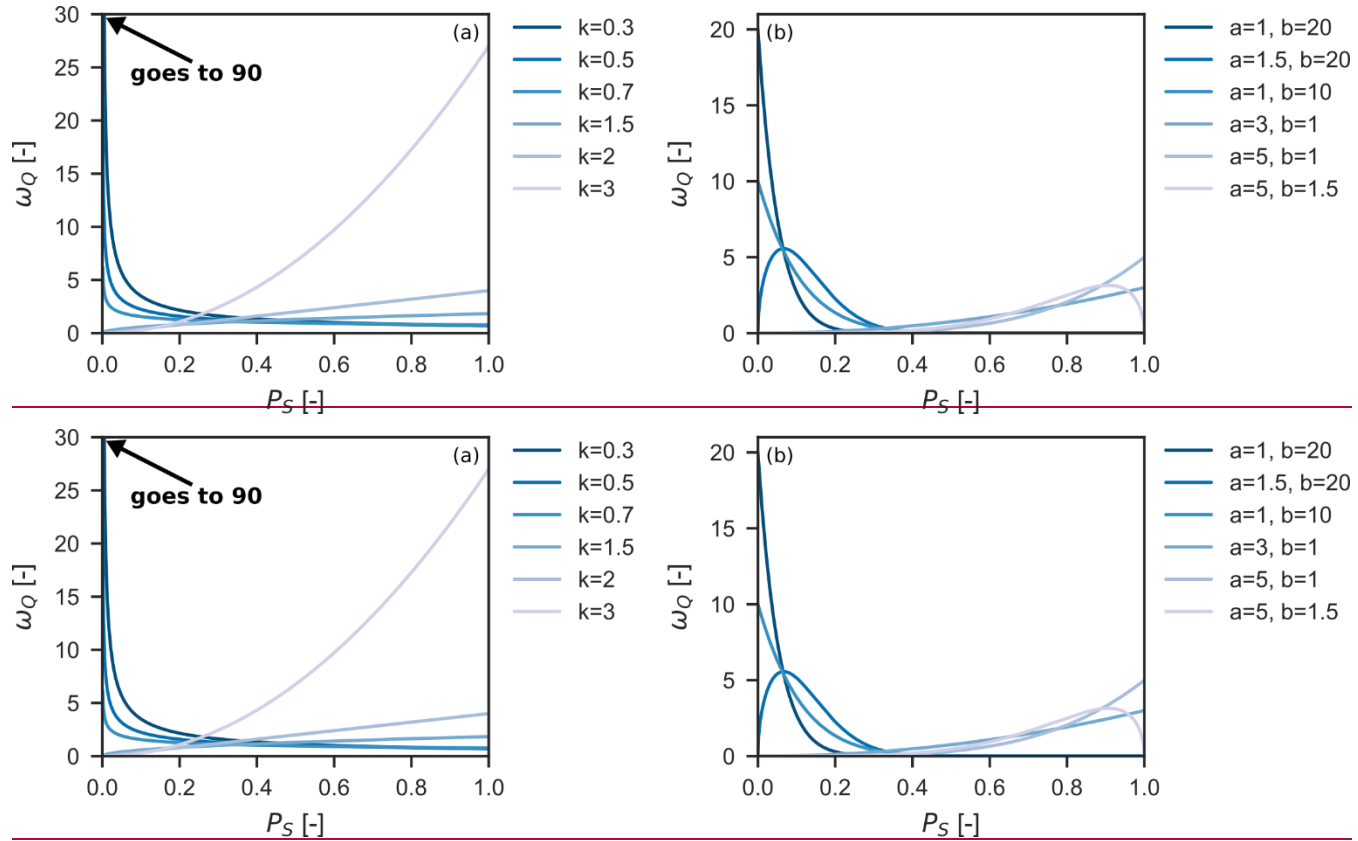
225   $$P_s(T,t) = \frac{S_T(T,t)}{S(t)}$$

(2)

and the corresponding cumulative power law distribution function:

$$\Omega_Q(T,t) = P_s(T,t)^{k_Q}$$

(3)

230 ~~wherewhere~~ where T is the water age (day), t is the time step (day), $\omega_Q(T,t)$ is the probability distribution function of the hydrologic flux, $\Omega_Q(T,t)$ is the cumulative probability distribution function), $S_T(T,t)$ is the cumulative age-ranked storage (mm), $S(t)$ is the soil water content (mm) and $P_S(T,t)$ is the cumulative probability distribution of the storage.

235 **Figure 2** Storage selection with different parameters illustrated for power law distribution function (a; see Eq. (1)) and Kumaraswamy distribution function (b; see Eq. (3))

As a second distribution function, we employ the Kumaraswamy distribution (Kumaraswamy, 1980). With two parameters a_Q and b_Q, the Kumaraswamy distribution provides a greater flexibility than a power law distribution (Fig. 2b). The Kumaraswamy distribution function is formulated as:

240 $$\omega_Q(T,t) = a \cdot b \cdot P_s(T,t)^{(a_Q-1)} \cdot \left(1 - P_s(T,t)^{a_Q^{(b_Q-1)}}\right)$$

(4)

and the corresponding cumulative Kumaraswamy distribution function:

$$\Omega_Q(T,t) = 1 - \left(1 - \left(P_s(T,t)\right)^{a_Q^{b_Q}}\right)$$

(5)

245 Generally, any distribution function might be used as long as a closed form (i.e. probabilities integrates to one) is available (Harman, 2015). We apply the fractional SAS function type (fSAS; van der Velde et al., 2012) and solve the SAS equations for each hydrologic flux Q. To solve the SAS functions, we provide three numerical schemes with fixed time steps: (i) deterministic (i.e. solving SAS equations for each flux in a sequential order), (ii) explicit Euler and (iii) explicit Runge-Kutta fourth-order. Transport processes can be defined for conservative and non-conservative

250 solutes:

- Stable water isotopes oxygen-18 (^{18}O) and deuterium (^{2}H): Isotopic fractionation is not yet considered.
- Bromide and chloride: Evapoconcentration, sorption processes and partitioning of root uptake are included.
- Nitrate: Biogeochemical processes denitrification (Kunkel and Wendland, 2012), nitrification, soil nitrogen mineralization and nitrogen uptake by crops are implemented.

255 Again, we refer to the online documentation of RoGeR for detailed information (Schwemmle, 2023). The following routines are implemented, and we refer to the module and declare whether the module is tested or testing is still ongoing:

- Solute transport and water ages (*transport.py* and *sas.py*; testing is complete)
260 - Nitrogen cycle (*nitrate.py*; testing is ongoing)

3 Test cases for continuous development, computational performance and energy usage

RoGeR uses unit tests and continuous integration to test and ensure technical functionality (see Table 1). Additionally, we use test cases for continuous development. The idea of these test cases is to guarantee predictive consistency and to track advances in model development (i.e. comparison between model versions). We run the test cases with model

265 parameters that cover a wide range of common parameters and perform simulations with different input data. In contrast to unit tests, the execution time is longer and depends on the number of time steps covered by the input data. The results (see Sect. S1) can be compared to future versions of RoGeR.

Table 2 Hardware specifications of computational benchmarks

	Notebook	Cluster node
CPU	Intel® Core™ i7 @ 2.60 GHz (four physical cores)	2 x Intel® Xeon® E5-2680v4 (Broadwell) @ 2.40 GHz (28 physical cores)
TDP[1] of CPU	45 Watt	280 Watt
RAM	8 GB DDR3	128 GB DDR4
GPU	-	Nvidia Tesla K80 (12 GB GDDR5 memory)
TDP[1] of GPU	-	300 Watt
Software stack	GNU 8.1, Open MPI 4.1.3, HDF5 1.12.2, roger 3.0	GNU 9.2, Open MPI 4.1.3, HDF5 1.12, CUDA 11.4, roger 3.0

^{1}Total power draw
270   ^{2}Power usage efficiency

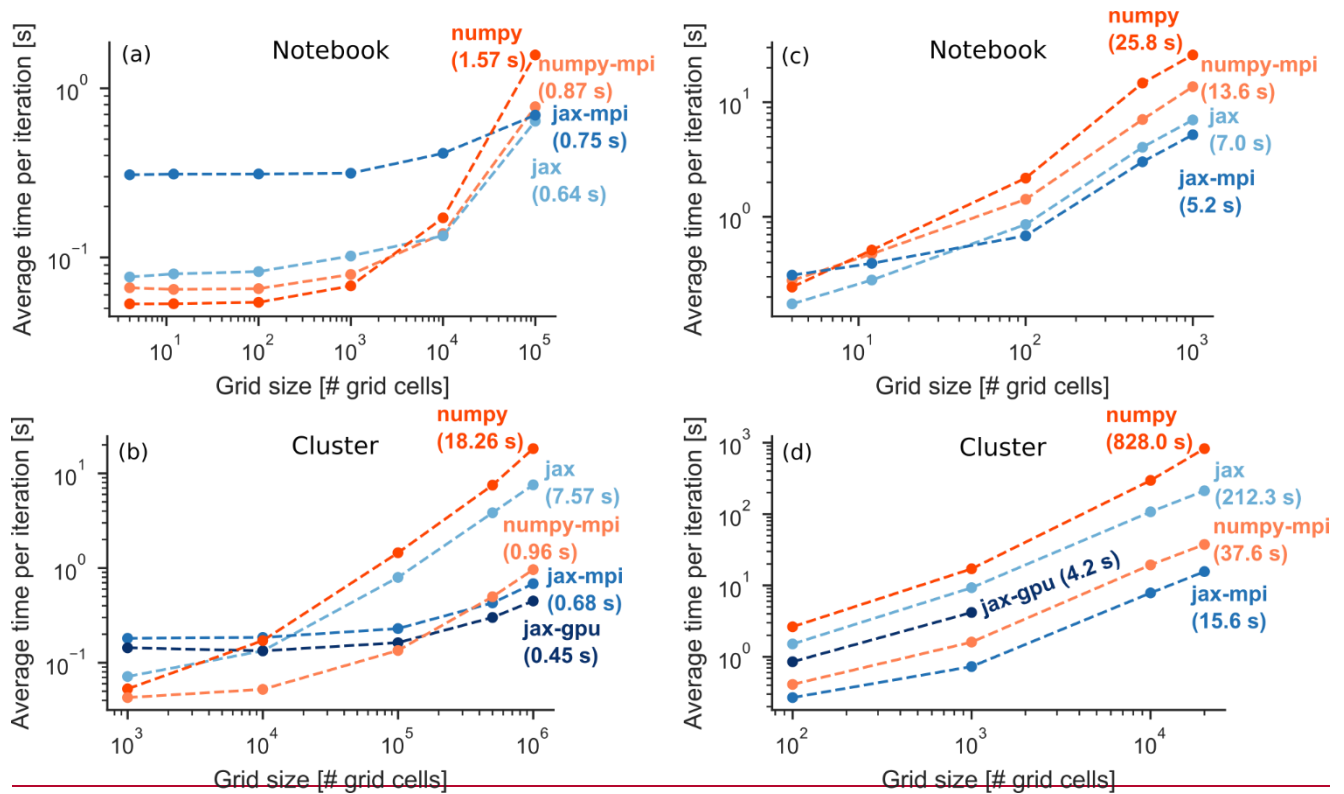



Figure 3 ~~Runtime performance of computational back-ends for the RoGeR-SVAT type model (a, b) and for the RoGeR-SVAT-~~
~~^{18}O type transport model (c, d). Note that, number of grid cells represents the two horizontal spatial dimensions (e.g. longitudes~~
275   ~~and latitudes). The total number of elements is greater for transport models due to additional age dimensions and can be derived~~
~~by multiplying the number of grid cells (i.e. two spatial dimensions) with the number of water ages (e.g. 1500). SVAT model used~~
~~100 iterations and SVAT-^{18}O transport model used 20 iterations.~~

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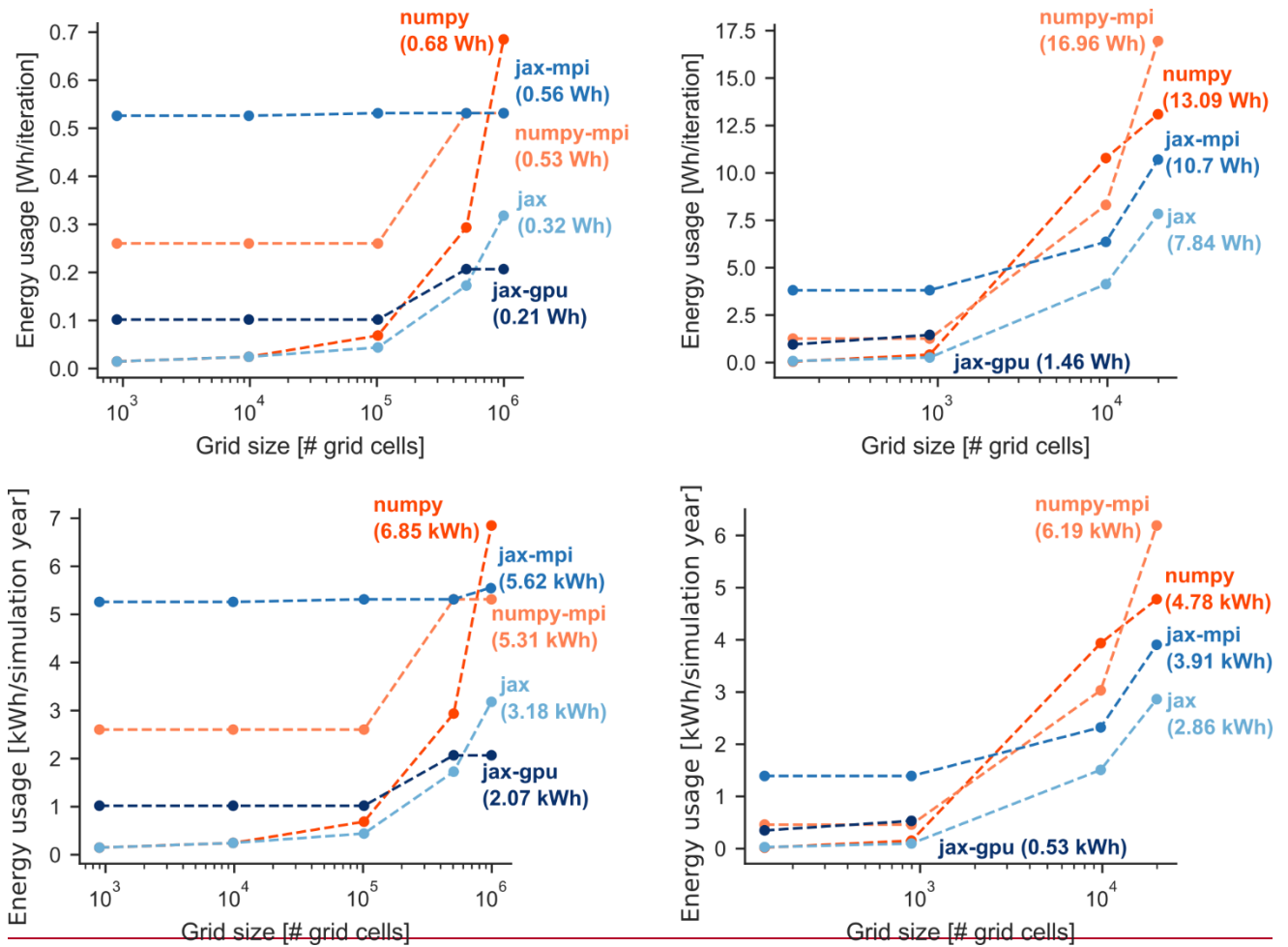
High-level programming languages such as Python still have the reputation of being comparatively slow. We profiled the computation time and energy usage using the five back-ends (see Sect. 2.1.2). For the profiling, we used two different hardware specifications representing commonly available computing resources and high-performance computing (HPC) resources (Table 2). We measured computation time and energy usage with a fixed number of iterations, but varying number of grid cells (Fig. 3).

Model parameters are the same for each grid cell. Figure 3 shows that for small modelling experiments (< 1000 grid cells), the numpy back-end performs equally well ~~than~~as the other back-ends. Parallel computation improves computational speed up only for intermediate to larger modelling experiments (> 1000 grid cells), provided that a greater number of CPU cores are available. Computation on a single GPU device is faster than on multiple CPUs for the RoGeR-SVAT type model, while multiple CPUs (numpy-mpi and jax-mpi) are faster than a single GPU device for the RoGeR-SVAT-^{18}O type model. However, a major requirement for GPU computing is that the modelling

295 experiment fits into the GPU memory ($< 10^6$ grid cells). A solution to the memory limitation would be the usage of multiple GPU devices.
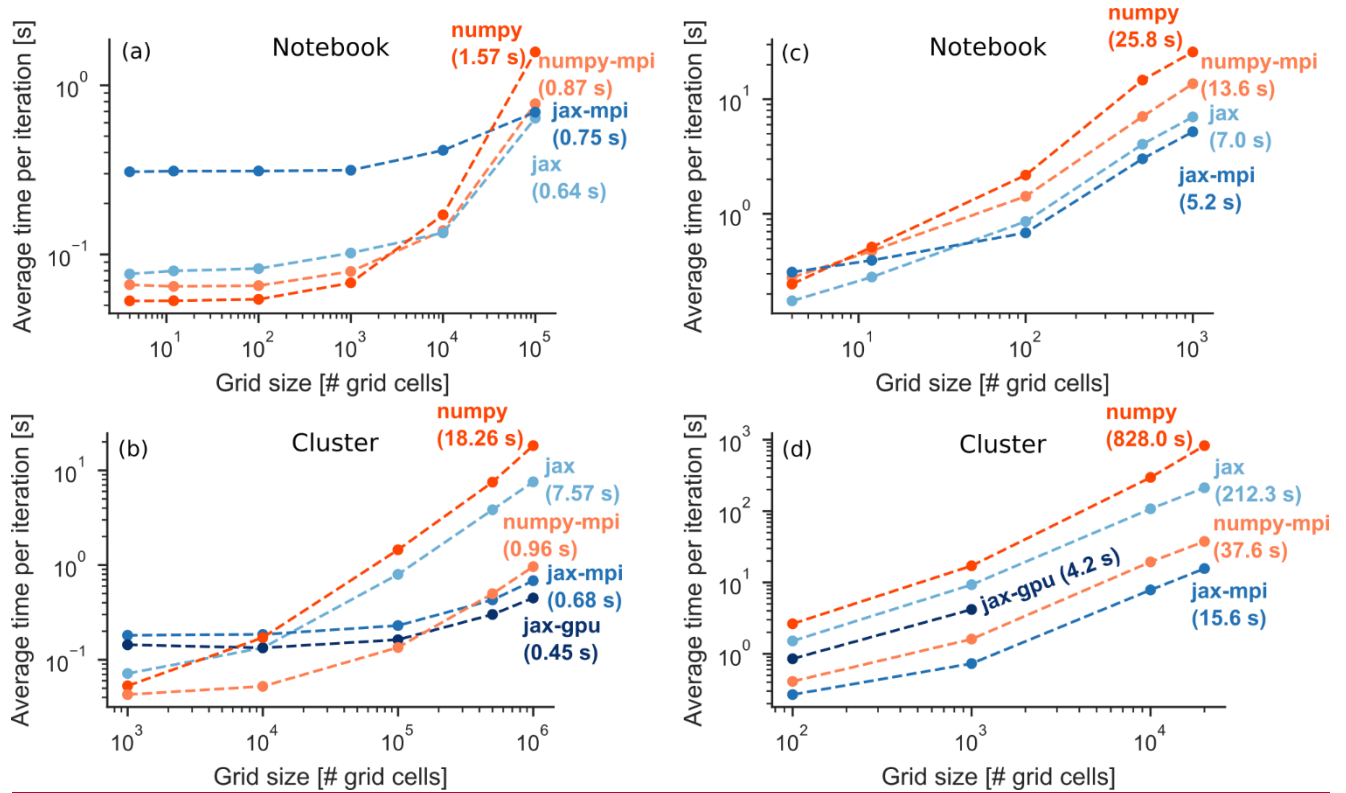
Figure 3 Runtime performance of computational back-ends for the RoGeR-SVAT type model (a, b) and for the RoGeR-SVAT-^{18}O type transport model (c, d). Note that, the number of grid cells represents the two horizontal spatial dimensions (e.g. longitudes and latitudes). The total number of elements is greater for transport models due to additional age dimensions and can be derived by multiplying the number of grid cells (i.e. two spatial dimensions) with the number of water ages (e.g. 1500). SVAT model used 100 iterations and SVAT-^{18}O transport model used 20 iterations.
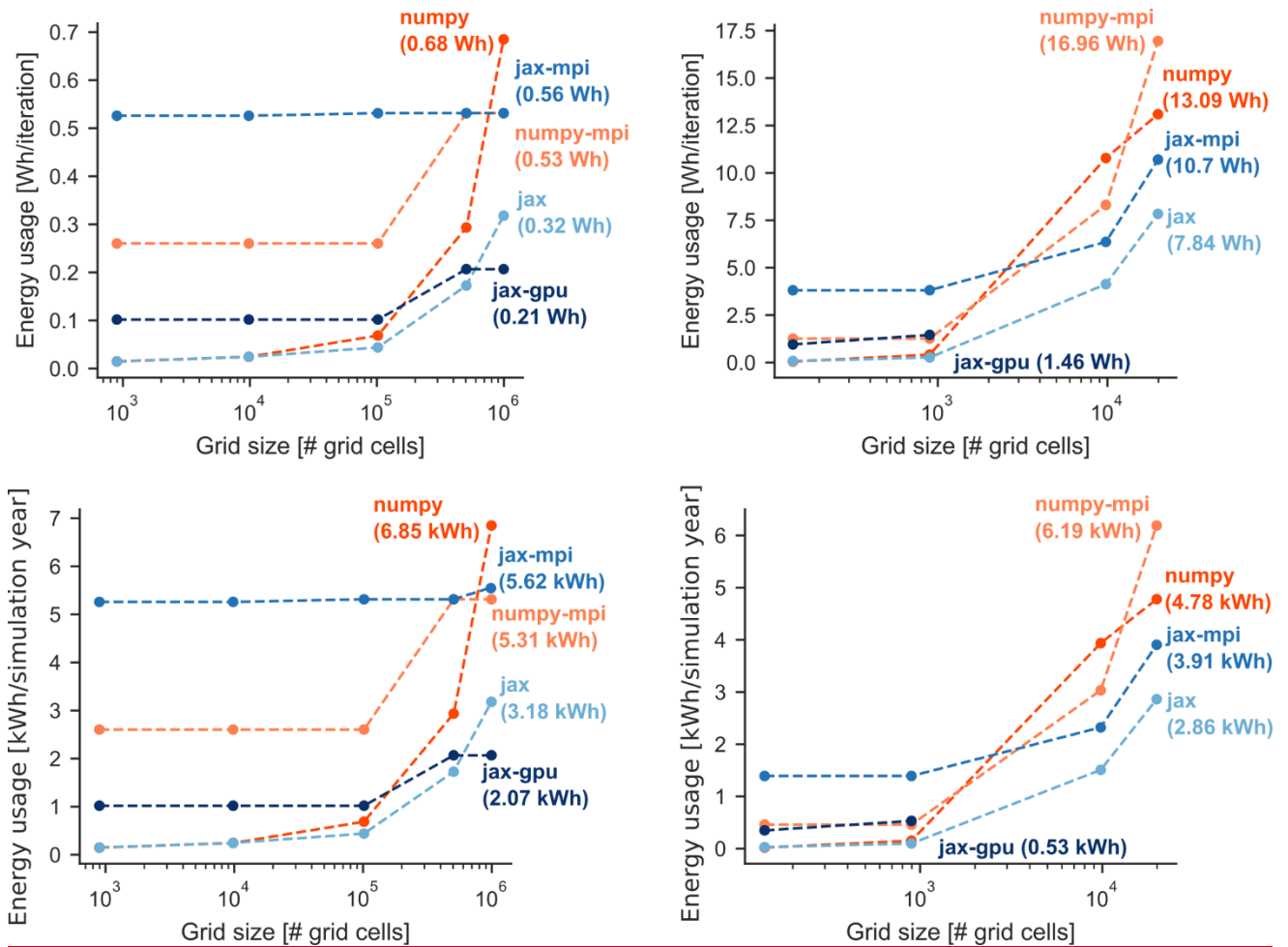
Figure 4 Energy usage of computational back-ends on a cluster node for the RoGeR-SVAT type model (a, b) and for the RoGeR-SVAT-^{18}O type transport model (c, d)

HPC consumes more energy than running computations on a notebook. Depending on the energy source, HPC contributes differently to climate warming (Lannelongue et al., 2021). In order to raise awareness about the energy usage in HPC context and to provide information for a sustainable allocation of computational resources, we profiled the energy usage of RoGeR in an HPC context (see Table 2). Based on the profiling of computation time, we calculated the energy usage of the five back-ends using the method proposed by Lannelongue et al. (2021). The results (Fig. 4) show that using multiple CPUs (numpy-mpi and jax-mpi) consumes more energy than other back-ends. Using a single GPU device decreases energy usage, while computation time still competes with multiple CPUs (cp. Fig. 3). For small and intermediate modelling experiments, single CPU (numpy and jax) back-ends use less energy than other back-ends. With these results, we aim to support efficient and sustainable allocation of computational resources. We suggest that computation time and energy usage should be considered equally for the allocation.

4 Application: Soil water balance, ¹⁸O transport and water age statistics of a three-year period

To demonstrate the capabilities of RoGeR, we present a simple application example. We simulate the soil water balance and fluxes and ¹⁸O fluxes of ~~a flat rectangular grassland (7200 m²~~the Eberbaechle catchment (1.54 km² with a resolution of 25 ~~m²~~m x 25 m) for a time period of three years. The input data was retrieved from the database WeatherDB, which provides data from stations operated by Deutscher Wetterdienst (DWD) tailored to the required format of RoGeR (Schmit, 2022). We
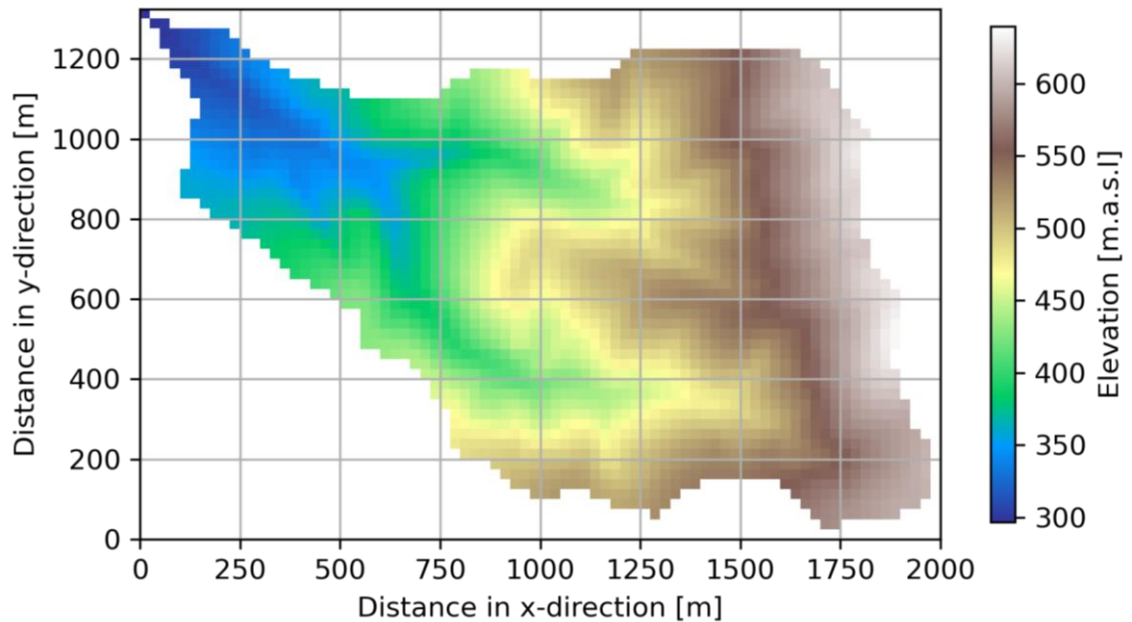
Figure 5 The Eberbaechle catchment used for the application example. The Further catchment properties used as model parameters are shown in Figs. S28 – S39. The coordinates of the catchment outlet are 47°57'24"N 7°49'48"E.

selected the DWD station at Freiburg airport (station ID: 1443) to obtain precipitation, air temperature and potential evapotranspiration data from November 2019 to October 2022. Since DWD stations do not measure solute concentrations in precipitation, data for ¹⁸O in precipitation has been generated by a sinusoidal function with random variation for amplitude and offset (Allen et al., 2018; amplitude=4.3±0.5 [‰], offset=-10±0.5 [‰] and phase=60 [days]). In order to ~~represent~~set the ~~local soil characteristics and their spatial heterogeneity, we randomly generated~~values for the model parameters ~~for each grid cell with typical parameter ranges provided~~listed in Table 3~~.~~, we used the soil map BK50 (Regierungspräsidium Freiburg, Landesamt für Geologie, Rohstoffe und Bergbau), LIDAR data (Landesvermessungsamt Baden-Württemberg), ATKIS DLM25 (Landesvermessungsamt Baden-

335 Württemberg). Additionally, we assumed a deep groundwater table implemented through a high hydraulic conductivity of the bedrock (see Table 3). SAS parameters for the selected power law distribution function are assumed to be spatially and temporally constant for each hydrological process and grid cell. We assigned k=0.12 to soil evaporation and capillary rise, k=0.35 to transpiration, k=21.5 to percolation of root zone and k=31.5 to percolation of subsoil. Thus, soil evaporation capillary rise, and transpiration have a preference for younger water, 340 while percolation processes have a preference for older water (see Fig. 2a).

Table 3 Model parameters for the Eberbaechle catchment

Hydrological model parameter	Symbol	Unit	Range of parameter values
Land use/Land cover	lu_id	-	Grass, forest, sealed surface, agriculture
Surface sealing	$sealing$	-	0 - 1
Soil depth	z_{soil}	mm	200 - 1000
Length of vertical macropores	l_{mpv}	mm	0 - 800
Density of vertical macropores	ρ_{mpv}	m^{-2}	0 - 200
Air capacity of soil	θ_{ac}	-	0.06 - 0.14
Plant available field capacity of soil	θ_{ufc}	-	0.1 - 0.2
Permanent wilting point of soil	θ_{pwp}	-	0.09 - 0.18
Saturated hydraulic conductivity of soil	k_s	mm h^{-1}	10.4 - 125
Hydraulic conductivity of bedrock	k_f	mm h^{-1}	2500[a]
Offset for air temperature	TA_{offset}	°C	-2.5 - -0.4
Weighting factor for potential evapotranspiration	PET_{weight}	-	0.73 - 1.06
Weighting factor for precipitation	$PRECIP_{weight}$	-	1.0 - 1.27

[a] results in free drainage

In Figure 56, we display the time series of hydrologic fluxes and soil water content with the corresponding ^{18}O signature and water age distributions of a single grid cell. The temporal pattern exhibits that soil water content and 345 travel times of hydrologic fluxes can be related. This pattern emphasizes the interlinkage between hydrologic states and transport velocities of solutes (Hrachowitz et al., 2016). Figure 67 shows the cumulative distributions of soil hydrologic fluxes, soil water content, δ^{18}O signals and medianaverage water ages at four different dates with different soil water content conditions. Soil water content is wetter at 9th December10th February 2021 and drier at 8th13th August 2022 while the other two dates represent the transition between drier and wetter conditions. The cumulative 350 distributions of δ^{18}O signals and medianaverage water ages reveal differences for these different soil water content conditions. The δ^{18}O signals display distinct differences between the considered fluxes and soil water storage. Moreover, spatial variation is more distinct for soil water storage and percolation than for soil evaporation and

transiration. The ~~median~~average water age exposes a more general pattern. For drier conditions, ~~median~~average water age is older, whereas for wetter conditions median water age decreases.

355 The primary objective of the example is to demonstrate the capabilities of RoGeR. Therefore, we kept the complexity of the example at a simple level. Although a comparison between simulations and observations is important to evaluate the fidelity of the model, we do not provide such a comparison here. Instead, we refer to Schwemmle and Weiler (2023) for an in-depth evaluation of RoGeR using measurements from a grassland lysimeter site. Since the development of RoGeR as scientific software started recently and is still ongoing, further evaluation of RoGeR will 360 be addressed in the future.
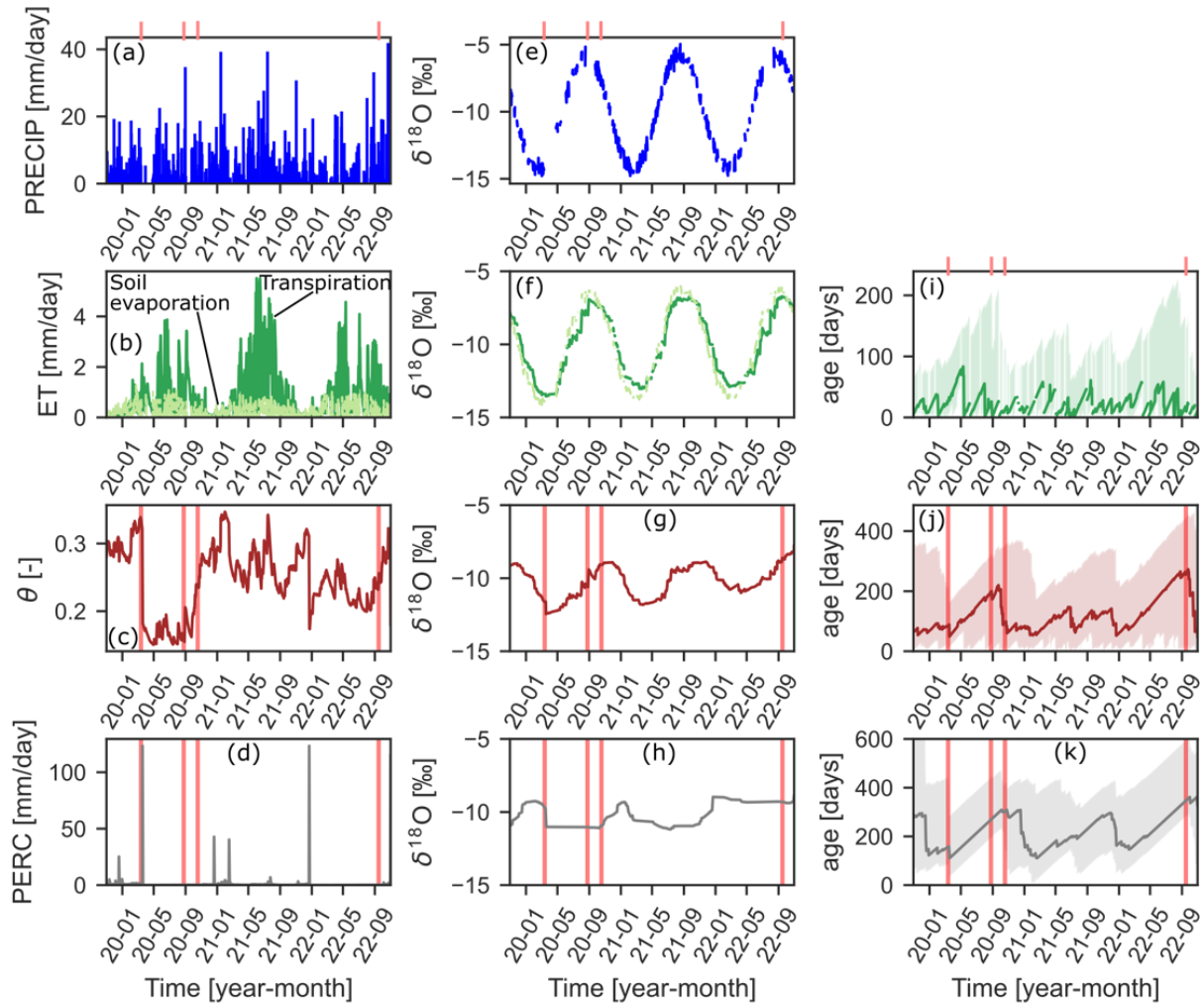
Figure 6 Simulated fluxes and soil water content (a-d), corresponding $\delta^{18}O$ signal (e-h) and corresponding 10th, 50th and 10th percentile of water ages (i-k) of a single grid cell. Vertical red lines indicate the four different dates from Figure 6. Power law
365 distribution function serves as SAS function (SAS parameters: $k_{evap\text{-}soil}=0.2$, $k_{transp}=0.5$, $k_{perc\text{-}rz}=1.5$, $k_{perc\text{-}ss}=1.5$; see Figure 2)
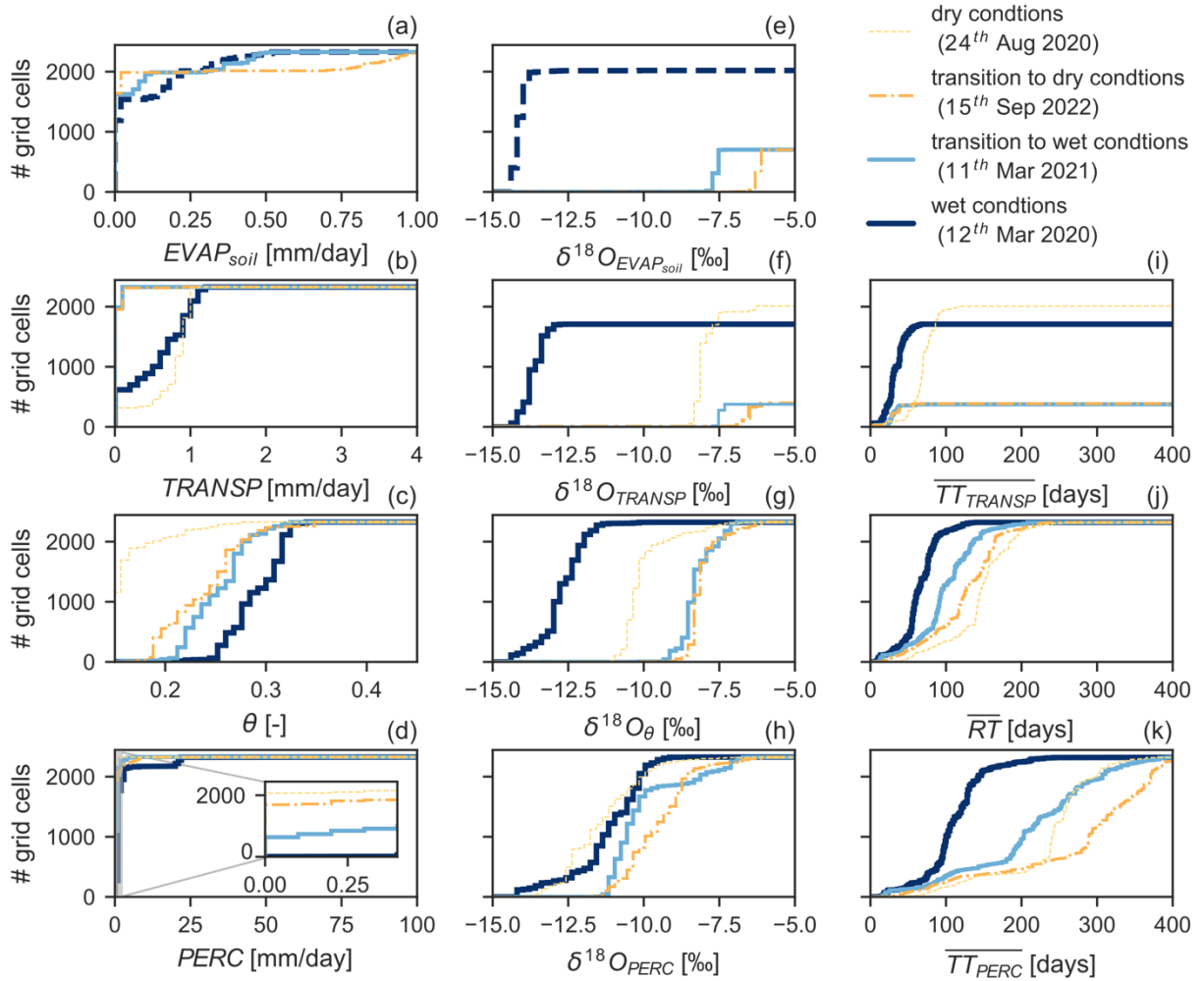
Figure 7 Cumulative distributions of simulated fluxes and soil water content (a-d), corresponding $\delta^{18}O$ signal (e-h) and the corresponding average travel time and average residence time (i-k) of the Eberbaechle catchment (1.54 km^2) at four different dates (transition to dry, dry, transition to wet and wet conditions)

The simple application example demonstrates the potential of RoGeR for a combined quantification of the water balance and solute mass balance. The example focusses on vertical soil hydrological processes and a conservative tracer, but this is just an excerpt of the toolbox. Other processes (e.g. lateral subsurface runoff, different SAS function; see Sect. 2.2 and 2.3) or other tracers (e.g. bromide; see Sect. 2.3) could also be considered and implemented.

~~**Table** Lower and upper boundaries used for random generation of parameter grids~~

~~Hydrological model parameter~~	~~Symbol~~	~~Unit~~	~~Parameter boundaries~~
~~Land use/Land cover~~	~~lu_id~~	~~-~~	~~grassland~~
~~Density of vertical macropores~~	~~ρ_{mpv}~~	~~m^{-2}~~	~~50 – 100~~

Length of vertical macropores	l_{mpv}	mm	200 – 500
Soil depth	z_{soil}	mm	1000 – 1200
Air capacity of soil	θ_{ac}	-	0.08 – 0.12
Plant available field capacity of soil	θ_{ufc}	-	0.08 – 0.12
Permanent wilting point of soil	θ_{pwp}	-	0.18 – 0.22
Saturated hydraulic conductivity of soil	k_s	mm h^{-1}	5 – 15
Hydraulic conductivity of bedrock	k_f	mm h^{-1}	2500[a]

[a]results in free drainage
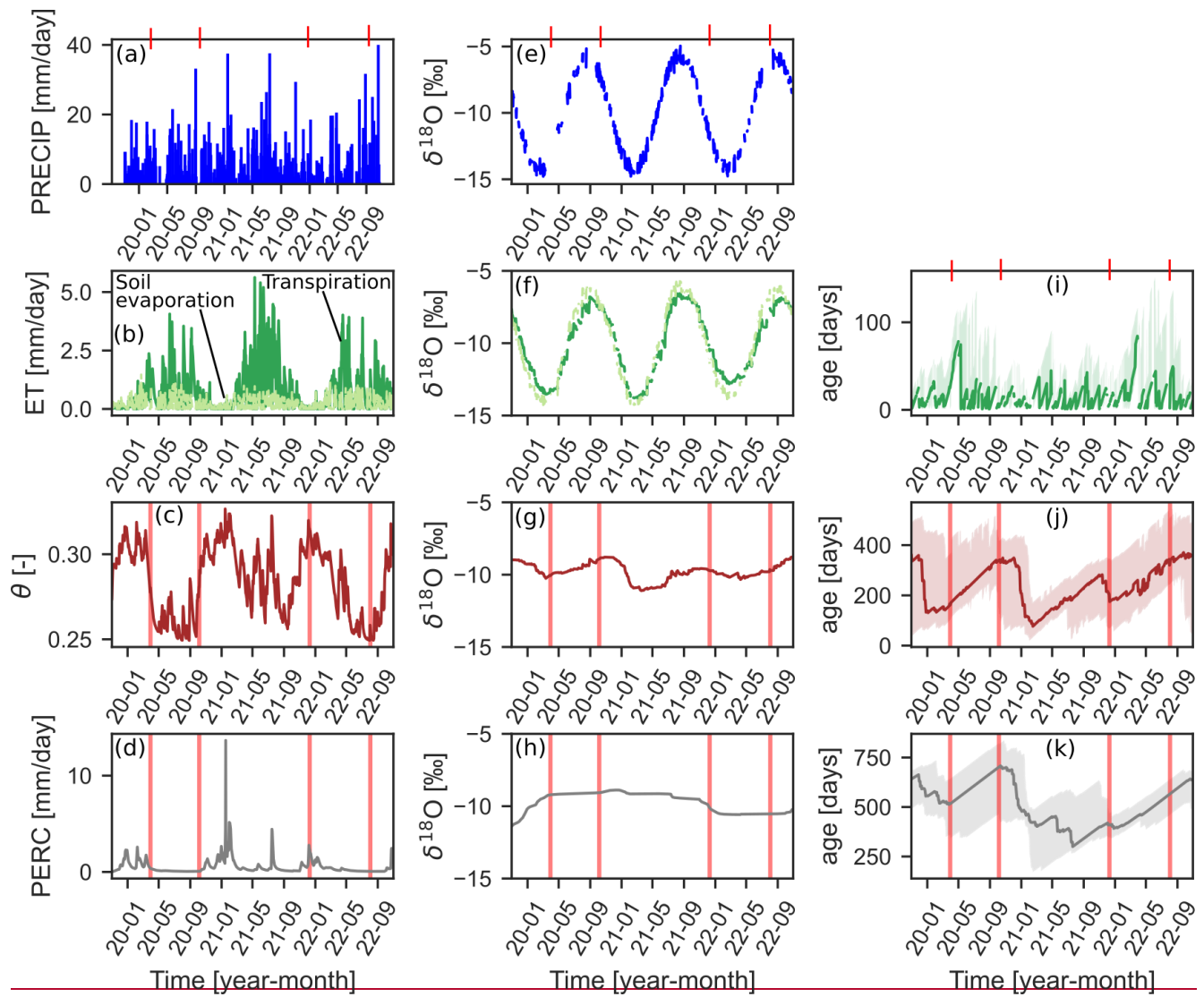
Figure Simulated fluxes and soil water content (a-d), corresponding δ¹⁸O signal (e-h) and corresponding 25th, 50th and 75th percentile of water ages (i-k) of a single grid cell. Vertical red lines indicate the four different dates from Figure 6. Power law distribution function serves as SAS function (SAS parameters: $k_{evap\text{-}soil}$=0.1, k_{transp}=0.3, $k_{perc\text{-}rz}$=2, $k_{perc\text{-}ss}$=3; see Figure 2)

 5 Summary and outlook

The development of the process-based hydrological toolbox RoGeR followed open-source software guidelines (Sect. 2.1). We believe that such guidelines improve the reproducibility in computational hydrology. With the modular code

385 structure (Sect. 2.1.1) and the good readability of Python code, RoGeR is intended to be easy to use (i.e. usable by programmers with little experience) and to be easy to modify (i.e. modification and extension of the code). With using different computational back-ends, we maintained code readability without hampering computational performance

(Sect. 2.1.2). The five back-ends provide the opportunity to simulate anything between plot scale and the catchment scale with reasonable computation times. Especially, the GPU back-end has great potential to reduce computation

390   time and energy usage of catchment scale modelling experiments (Sect. 3).

In comparison to the publicly available hydrological models written in Python, we combined hydrological processes (Sect. 2.2) and solute transport based on SAS (Sect. 2.3). The combined representation enables the prediction of hydrologic states and fluxes and their corresponding solute concentrations including travel times. The simple application example considering the water balance and ^{18}O transport through the soil of a rectangular grassland the

395   Eberbaechle catchment showed plausible results. The RoGeR toolbox contains many processes to describe one dimensional hydrological processes (i.e. no lateral transfer between grid cells). The implementation of the lateral transfer between grid cells (i.e. routing schemes for surface and subsurface runoff) will be addressed in future releases. Surface runoff routing will be implemented using a hydraulic scheme. Subsurface runoff routing will use the approach of Steinbrich et al. (2016) which is based on the topographic slope and corresponding flow velocities. Moreover, we

400   suggest that future work may improve or extend the currently available process representations (e.g. gravity-driven infiltration and percolation; Demand and Weiler, 2021; Germann and Prasuhn, 2018) and further evaluation of RoGeR with measured data may provide insights on the strengths and weaknesses.

RoGeR contributes to a further diversification of the hydrological model landscape and the disagreement about process representation in the hydrological modelling community will continue (Weiler and Beven, 2015). In general,

405   an advantage of this diversification and disagreement is that many different approaches are available and, hence, a great flexibility to address different problems. On the other hand, the theoretical diversification is accompanied by technical diversification (e.g. different programming languages or different data formats) that lead to inconsistencies in the application. We suggest that the diverse hydrological model landscape might benefit from focussing on constrained data interfaces of the models following common data conventions (Hallouin et al., 2022) and

410   implementing standardized model interfaces (Hut et al., 2022; Hutton et al., 2020). This would facilitate the integration of hydrological models in earth science models. Another advantage would be that multiple hydrological models could be compared more easily. Such a model comparison of RoGeR with other models, for example, with tRIBS (Ivanov et al., 2004a, b; Vivoni et al., 2004), VIC (Hamman et al., 2018) or mHM (Samaniego et al., 2010This would facilitate model inter-comparison and models could be integrated in earth science) may be useful to highlight

415   advantages and disadvantages of using RoGeR compared to other models.

Supplement. The supplement related to this article is available online at: https://doi.org/10.5194/gmd-2023-118-supplement

Data availability. The meteorological input data used in the application example has been retrieved from https://weather.hydro.intra.uni-freiburg.de/ (Schmit, 2022) and is available at https://github.com/Hydrology-IFH/roger/tree/main/examples/hillslope_scale/svat_distributed_tutorial.

Author contributions. MW conceived the idea of the hydrological model RoGeR. MW, HL, AS and RS conceptualized RoGeR. HL and AS developed the first model suites of RoGeR in Python. RS developed RoGeR as a software package with support from HL translating python code into a software package. RS wrote the first draft of the manuscript with contributions from all co-authors.

Competing interests. The authors declare that they have no conflict of interest.

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