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A REGIONAL HYDROLOGICAL SOIL MODEL FOR LARGE-SCALE APPLICATIONS: COMPUTATIONAL CONCEPT AND IMPLEMENTATION

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A parallelized large-scale regional hydrologic soil model (RHSM) is developed as a tool for large-scale unsaturated zone investigations. It is applied to simulate the temporal and spatial responses of the unsaturated zone and the regional water budget under the forcing of realistic precipitation and evaporation scenarios. The Richards equation is used to describe the flow movement in the vadose zone and is solved using a finite element code. The RHSM provides a way to deal with the enormous discretization demand of unsaturated flow simulation at regional scales. The relatively thin soil cover is modeled vertically by 1D line elements with adequate resolution, whereas the large lateral dimensions are modeled as coarser grid patches, the so-called influence areas. In order to achieve reasonable computation times for a single model run the independence properties of the RHSM are elegantly exploited to realize a relatively uncomplex code parallelization. The parallelized RHSM runs on Linux supported symmetric multiprocessing computers using the message passing interface (MPI). This implementation attains a high performance computation of regional scale hydro-system models. In an application study at the Beerze-Reusel drainage basin (Netherlands), a high resolution of variably saturation distributions and wet front movements are obtained for the anisotropic field using the parallel RHSM. An analysis of the computational speed-up demonstrates the performance gain of the parallel RHSM.

INTRODUCTION

A large-scale hydrologic model is an indispensable research tool for hydrologists to investigate regional hydrological features under the influence of global climate change, anthropogenic alteration, or land-use change in recent decades. In hydrological analysis, unsaturated flow simulation is important since the vadose zone constitutes the interface between hydrosphere and atmosphere and governs transfer of water and contaminants from the atmosphere to the subsurface. As such, soil moisture patterns influence recharge to groundwater. On a larger scale wet-dry patterns in soil may also have an effect on convective cells in the atmospheric boundary layer (Patton et al., 2005). Moreover, it was demonstrated in a modeling study by Clark et al. (2004) that rainfall locations and intensities can be influenced by the presence and size of a wet soil patch down to scales of 10-15 km. A recent example of successful large-scale hydrologic modeling is the Altamaha river drainage basin study (Aral and Gunduz, 2003; Gunduz, 2004). Other macroscale hydrological models include the VIC-3L model, which was used for the upper Mississippi river basin (U.S.) (Srinivasan and Lakshmi, 2005), and the Xi'anjiang model, which is used in China chiefly for stream flow computations (Ren and Yuan, 2005).

Many different approaches have been developed to model water movement in the unsaturated zone. They can be summarized as: 1) quasi-linear analysis; 2) Green-Ampt (GA) method; 3) kinematic wave approximation; and 4) perturbation method. Quasi-linear analysis was first presented by Garden (1958) and later generalized and applied by Philip (1968, 1992). The GA method, originally developed by Green and Ampt (1911) for a one-dimensional domain and a single infiltration period, was extended to a more generally applicable model by Mein and Larson (1973). A large-scale application of GA was carried out by Govindaraju and Corradini (2000). Ogden and Sahafian (1997) introduced the GA redistribution (GAR) technique to estimate the soil water distribution during transient rainfall. The comparison of their results with those computed by numerically solving a Richards model showed a high level of agreement and demonstrated the accuracy of GAR. The kinematic wave approximation, brought forward first by Lighthill and Whitham (1955), handles wetting and draining waves travelling downwards through unsaturated soils. More recently, this method was used by Smith (1983), Levy and Germann (1988), Singh (1997), and Troch et al. (2002, 2003). The perturbation method was developed by Prasad and Romkens (1982). Of these methods, the Richards equation remains the most widely accepted framework for soil water flow analysis e.g. (Milly, 1988; Schüze et al., 2005). The numerical implementation of the solution of the Richards equation has been detailed extensively by Segol, (1993) and Kolditz (2002).

At large scales a significant temporal diversification of soil moisture contents is observed due to the variability of meteorological variables such as precipitation and evapotranspiration. The coupling of hydrological models with regional climate models was therefore undertaken to investigate the linkages between both systems (Stamm et al., 1994; Walker and Houser, 2001; Hurk et al., 2004), the sensitivity of the hydrosystem to climatic conditions (Gedney and Cox, 2003), and the feedback of soil moisture content to local or regional climate systems (Yeh et al., 1994; Schaer et al., 1999).

Apart from the meteorological forcing, the spatial variability of soil properties needs to be considered. With sophisticated data sampling techniques and tools for data processing and management at hand, large-scale distributed modeling is becoming a more and more viable option despite its enormous demand for data and computational resources. More and more models

choose parallelization as a practical tool to solve massive and large scale problems. The parallel integrated hydrologic model ParFLOW was developed by Ashby and Falgout (1996). The model exhibits higher parallel efficiency in solving small problems compared to large problems. Overland flow simulation requires considerably more computational effort compared to other processors, causing low parallel inefficiency. Dawson et al. (1997) brought forward a parallel implicit cell-centered method for two-phase flow with a preconditioned Newton-Krylov solver. In Jones and Woodward's (2001) work, the parallel computation results show the effectiveness of the entire nonlinear solution procedure and parallel efficiencies. As for other models, the sequential hydrological model SWMS_3D was upgraded to a parallelized version by Hardelauf et al. (2007), and its reliability was tested and performance and efficiency was compared with a single processor run. Once the computation efficiency was improved by parallelization, more integrated hydrological models became possible. Kollet and Maxwell (2006) incorporated an overland flow simulator into the parallel three-dimensional variable saturated subsurface flow code ParFlow. In addition, the influence of groundwater dynamics on the energy balance at the land surface was studied using this integrated, distributed modelling platform (Kollet and Maxwell (2008)).

In this study, we give a detailed description of the implementation of a parallelized regional hydrological soil model or RHSM, and present a class of solvers developed for the parallel solution of Richards' equation, the model chosen for variably saturated flow simulation. The parallelized RHSM provides an approach that meets the required vertical discretization demands on the one hand, and keeps the computational efforts realistic on the other hand. Additionally, the lateral spatial variability of meteorological input or soil parameters can be incorporated into the simulation with an appropriate level of detail.

Notwithstanding the parallelization, the RHSM remains computationally intensive for models of the size of river basins, and this approach is not only necessary, but is an integral part of the concept. Parallel computing has two paradigms in general: message passing (<http://www.mpi-forum.org>) and shared memory (<http://www.ics.uci.edu/javid/dsm.html>). In message passing the individual parallel processes exchange data via the computer network. In the shared memory model, parallel processes access one publicly available memory and pass information by coordinated reading and/or writing of the information stored. As the message passing model possesses several advantages, e.g. easy programmability, scalability and portability, we use this paradigm in this study.

In the following we first give a detailed description of the parallelized RHSM and then cover some of the implementation features used within the GeoSys/RockFlow (GS/RF) software platform (Kolditz, 2004; Wang and Kolditz, 2007). We perform a benchmark test for the validation of this implementation and apply it to the Beerze-Reusel area in the Netherlands, where a large scale comprehensive soil property data base was available. Finally, the computational efficiency of the parallelized code is investigated by determining speed-up factors for an increasing number of processors.

MODEL THEORY

Conceptual model

The basic concept of the RHSM is the use of a local one dimensional soil column as an effective model segment that is represented by a mesh of vertical line (finite) elements that approximate the (essentially vertical) movement of water through the three dimensional unsaturated zone. This

one dimensional column approximation is assumed to be valid for a certain lateral extent, the so-called influence area of the vertical column. The influence area may be outlined by a polygon and may be viewed as a function of topography, vegetation, as well as lateral soil profile variability. The origin of the finite element meshes for flow computation is the weight center of the influence area, and its vertical discretization can be made a function of the thickness of each soil layer. Further refinement may also be required due to numerical reasons. This concept is shown in Figure 1. The top of the soil column represents the topographic surface and the bottom is, by definition, the groundwater table. In order to maintain this configuration, the elements can shrink or elongate according to the groundwater table variations. The RHSM itself is the spatial arrangement of the numerous soil columns connected laterally by their respective influence areas. An important assumption of this approach is that flow within soil columns is independent of neighboring soil columns, which neglects lateral flow and is strictly only valid for flat or mildly sloping areas. Lateral flow may be incorporated by the use of prism elements. However, in order to represent lateral flow for large scales reasonably well, the advantage of the coarser discretization using influence areas is lost.

Data model

In order to fill the conceptual RHSM with the parameter information, an interface to a data management system has to be created and integrated into the RHSM framework. The required information is as follows:

- Spatially distributed meteorological time series of precipitation, air temperature and sunshine duration.
- Land-use and vegetation maps.
- A digital elevation model.
- Influence areas as well as soil type profiles (should include a description of pressure-saturation and permeability-saturation relationships; see Figure 1).
- Contaminant concentrations and properties (for additional transport computations only).

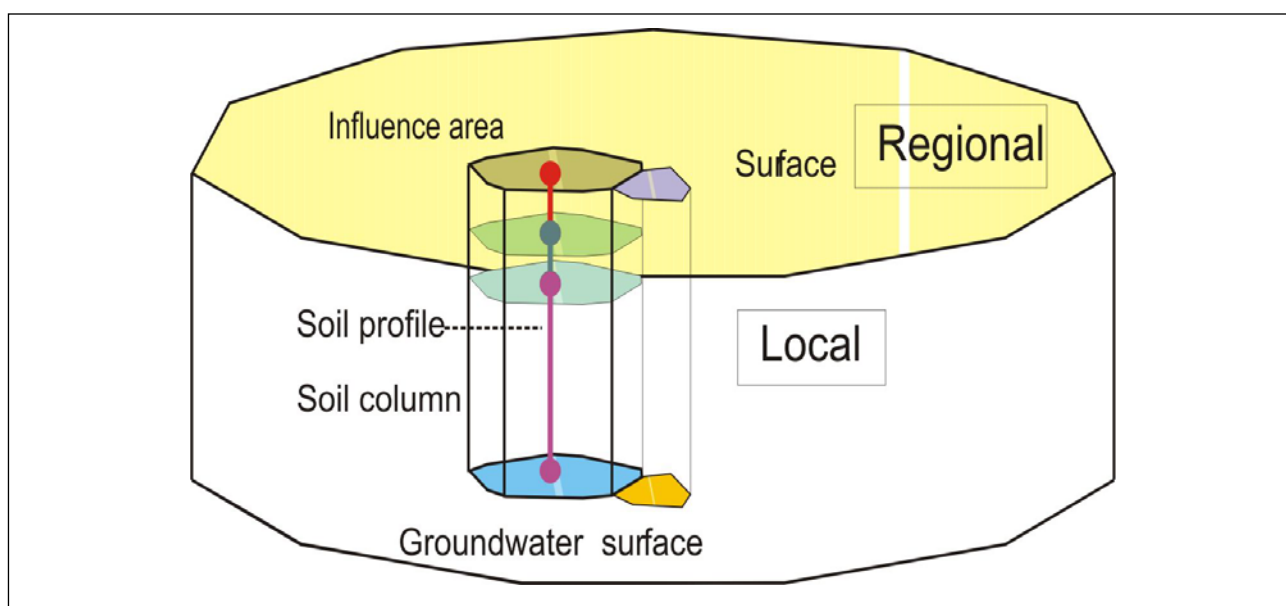


Figure 1. Illustration of the concept of the regional hydrologic soil model.

Mathematical model

The GS/RF software uses the Richards equation for unsaturated water flow computations. The Richards equation is obtained by combining Darcy's law with the law of mass conservation and the assumption that the air phase is at constant atmospheric pressure and not interfering with the water phase. Mathematically, the incompressible and non-deformable pressure-based Richards equation can be written as:

$$n \frac{\partial S}{\partial p} \frac{\partial p}{\partial t} - \nabla \cdot \left(\frac{k_{rel} \mathbf{k}}{\mu} (\nabla p - \rho \mathbf{g}) \right) = \frac{Q_p}{\rho} \quad (1)$$

in which n is the soil porosity, S is the soil water saturation, p is the soil water pressure, k_{rel} is the relative permeability, \mathbf{k} is the saturated permeability, μ is the water viscosity, Q_p is a source/sink term, ρ is the water density, \mathbf{g} is the gravitational acceleration, and t is time. Constitutive relationships describe saturation S as a function of (capillary) pressure and relative permeability k_{rel} as a function of S . The exact functional relationships may be obtained either from the empirical expressions given by van Genuchten (1980) or by an explicit description of soil water characteristic curves (SWCC). The SWCC provided in the available database define the functional relationships of $p(S)$ and $k_{rel}(S)$, neglecting hysteresis, with the effective saturation being

$$S_{eff} = \max \left(0, \frac{S - S_r}{S_{max} - S_r} \right) \quad (2)$$

where S_r is the residual saturation. The empirical functions for capillary pressure and relative permeability are given by,

$$p = \frac{\rho g}{\alpha} (S_{eff}^{1/m} - 1)^{1-m} \quad (3)$$

and

$$k_{rel}(S) = S_{eff}^{1/2} \left[1 - (1 - S_{eff}^{1/m})^m \right]^2 \quad (4)$$

where α and m are the so-called van Genuchten parameters.

We solve the Richards equation numerically by a Galerkin finite element method. Mass lumping is employed to improve solution convergence and stability behavior. For the time discretization, we use an adaptive time stepping with an embedded error control as given in Kavetski et al. (2001).

Model verification

The implemented solution procedure within GS/RF was verified by a direct comparison to the MIN3P software (Mayer et al., 2002). The comparison was based on a laboratory experiment with soil samples from the Elbe River where pulsed artificial rainfall was applied to a 0.25 m high soil column. The artificial forcing is illustrated in Figure 2 along with the temporal evolution of soil water saturation at three selected observation points ($z = 0.25, 0.1, 0.05$ m). Within the modeling exercises the hydraulic head at the bottom of the soil column was set to be constantly zero. As shown by the simulation, the solutions of GS/RF are in excellent agreement with those of MIN3P. Additional benchmark results for unsaturated zone water flow using GS/RF can be found in Kolditz et al. (2006).

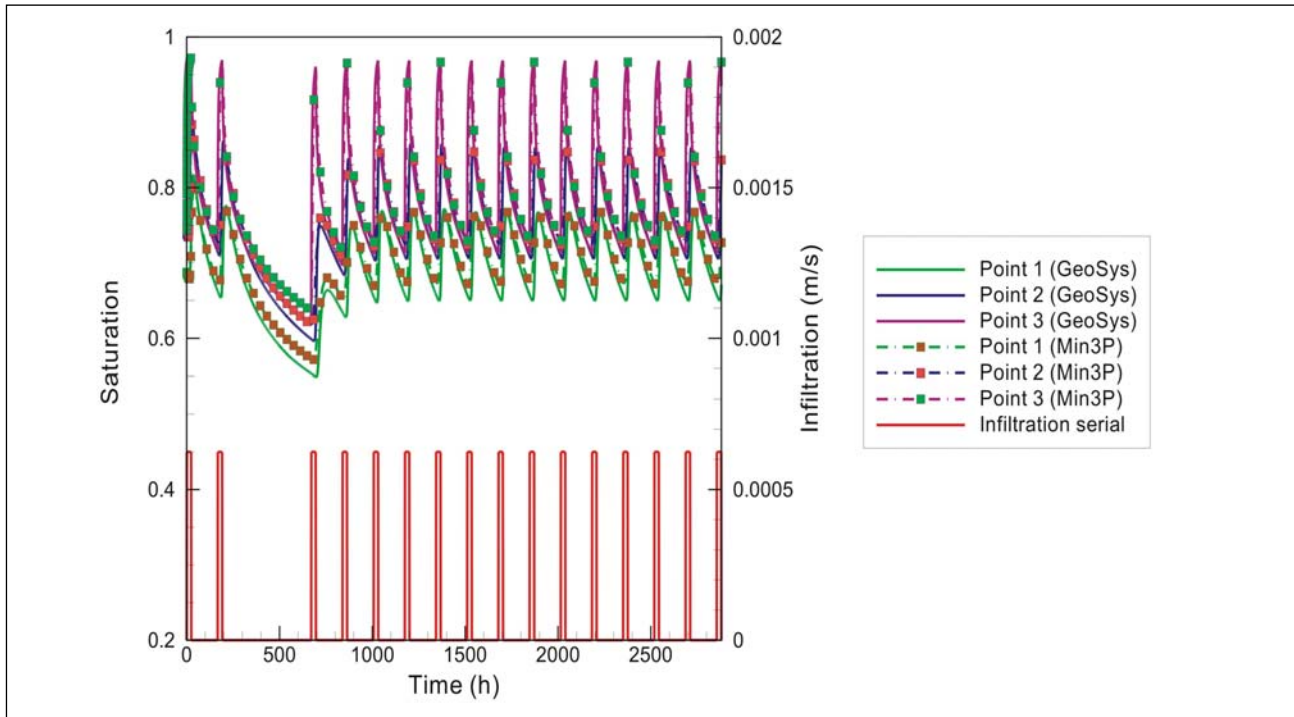


Figure 2. An inter-comparison of MIN3P and GS/RF for a transient Richards problem.

SOFTWARE CONCEPT

Object-orientated programming and implementation

Object-orientated programming understands the software as a collection of objects and their defined interactions. Hereby objects are instances of abstractly defined classes that contain both data (also called properties) and functions (also called methods) to manipulate this data. By this the encapsulation is achieved, as an object's properties can only be accessed by its own methods. Defined interaction between objects (also of objects belonging to different classes) is achieved by one object calling the other object's methods and vice versa. Another fundamental concept is inheritance, where new classes may be defined by inheriting properties and methods from already existing classes. If properly designed, these concepts achieve two of the big advantages of object-orientation: easy extendibility of the software's functionality and code-reuse ability.

In the GS/RF software individual processes are instances of the process class. The RHSM discerns between two process types: a regional (Richards) process and a local (Richards) process as depicted in Figure 1. The regional process defines a regional problem that also comprises components of the boundary condition (BC) object, initial condition (IC) object, source term (ST) object and equation object in its overall solution procedure. The single regional process also collects the geometric diversities inherent to the given local Richards processes. In other words, the definition of the regional Richards process also includes the arrangement of local Richards processes.

Database organization

The RHSM has an interface to a geographic information system, which stores the spatially related data such as influence area location and shape, as well as soil parameter profiles. As the spatial structure of the soil layer may contain numerous different soil types that may vary in complex patterns, an efficient organization of such databases is indispensable. Figure 3 shows the database organization of the RHSM using the ArcGIS software.

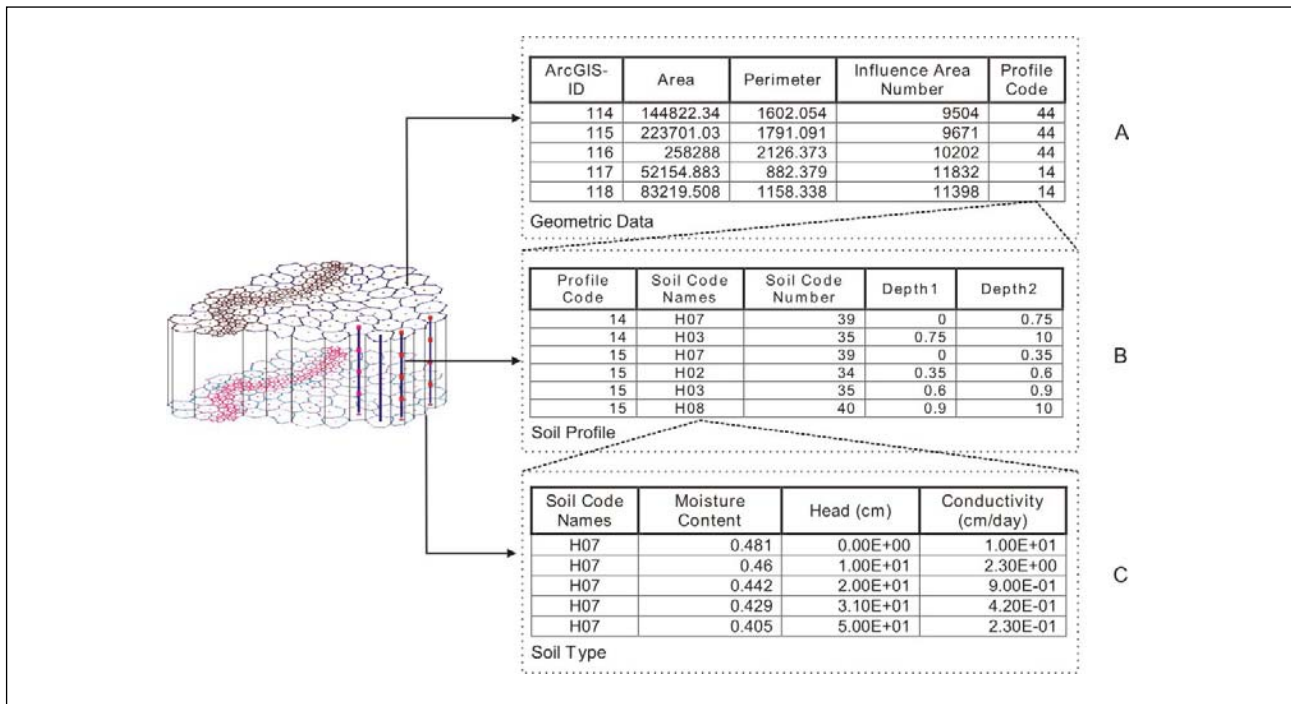


Figure 3. Database organization of RHSM. Data is grouped into (A) topographic information, (B) soil profile, and (C) soil type.

Topographic information. This table contains points and polygons that hold influence area locations and shapes. It is linked to vertical information via the soil profile code. (see Figure 3-A.)

Soil profiles. The soil profile table contains the vertical sequence of soil types with their respective thickness. This table is linked to soil property data via soil code names. (see Figure 3-B.)

Soil types. This basic table holds information on soil type flow characteristics (see Figure 3- C). These can either be given by SWCC or by van Genuchten parameters.

Parallelization approach

In this section the sequence of processing steps for the parallelized RHSM is outlined. The Algorithm 1 illustrates the pseudo-code of distributing the job of N loaded local Richards processes and their solution

The GS/RF software is coded in the C++ programming language, which makes inter-processor communication conveniently achievable by adding MPI statements to source code. The MPI implementation used within GS/RF is <http://www-unix.mcs.anl.gov/mpich1>. Since each local Richards process is independent, there is no data exchange necessary during computation execution. However, the job scheduling and computational load distribution is handled by the parallelized code. For any given number, P ($P > 0$), of processors a simple round-robin approach is used: For a total of N local Richards processes we have $P-1$ groups of $\nu = [N/P]$ local Richards processes, which have to be calculated sequentially by a single processor. The remaining $mod(N,P)$ local Richards processes are distributed to the P^{th} processor. Upon completion of all local Richards processes message passing is carried out to forward the results to the regional Richards process. The parallel scheduling is depicted in Figure 4 and a pseudo-code skeleton is provided in Algorithm 2.

Algorithm 1. Skeleton of regional soil model.

```

Time loop of the simulation
  if Regional and Richards
    Create local Richards processes
    for local Richards  $k$  ( $k \in [1, N]$ )
      Load local Richards  $k$ : BC, IC, ST
      Solve the non-linear equation for Richards  $k$ 
    end for
  end if
    
```

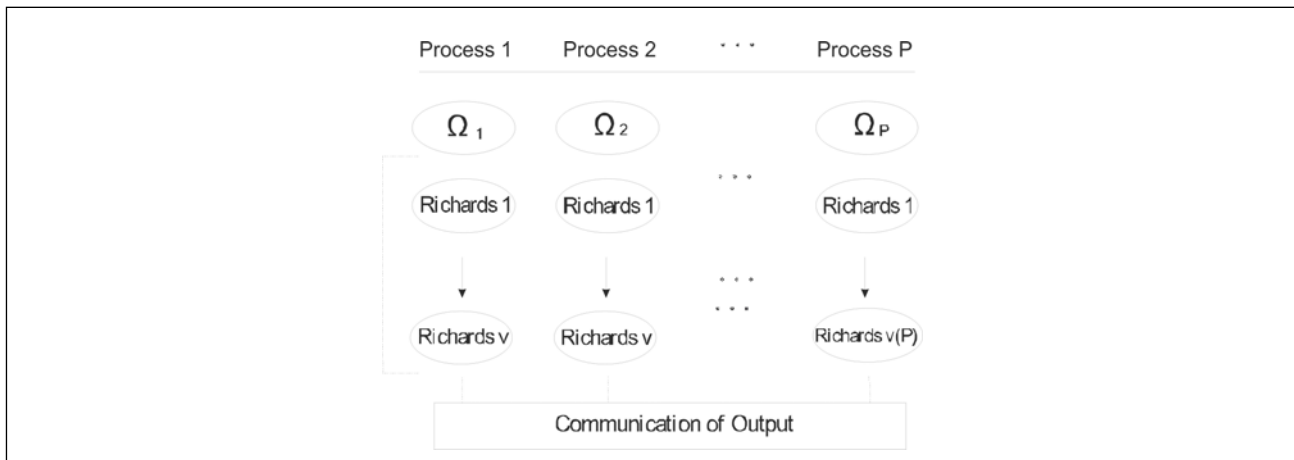


Figure 4. Schematic diagram of the parallel process execution of the RHSM.

Algorithm 2. Skeleton of parallel computation.

```

Time loop of the simulation
  if Regional and Richards
    Create local Richards process
    Divide the set of total Richards processes into  $P$  groups
    Start of parallel processing of group  $i$ ,  $i \in [1, P]$ 
    for local Richards  $k$  ( $k \in [1, \nu(i)]$ ) in group  $i$ 
      Load local Richards  $k$ : BC, IC, ST
      Solve non-linear equation for local Richards  $k$ 
      Communicate the computation result to the global space
    end for
    End of parallel processing of group  $i$ 
  end if
    
```

Test environment

The application study and preliminary testing of the parallelized RHSM implementation was carried out on a small Linux cluster consisting of four dual-cpu nodes. Each node is equipped with two AMD Opteron 248 processors and four GB of memory. The nodes are connected by a gigabit ethernet. The system has a theoretical peak performance of 35.2 GFlop/s.

APPLICATION OF THE PARALLELIZED RHSM TO THE BEERZE-REUSEL AREA

Geomorphological setting of the basin

The Beerze-Reusel drainage basin belongs to the province of North Brabant which is located in the southern Netherlands. A geographic overview of the basin is given in the bottom inset of

Figure 5. The shallow subsurface geology mainly consists of sandy deposits formed during the Pleistocene. The generally flat region gently slopes towards the direction north/northeast, and spans an elevation range between 45 m MSL (Mean Sea Level) to 3.7 m MSL. There are several aeolian sand ridges of a few meters in height striking west-east. These ridges have a large impact on the morphology of the stream valleys, as they are situated transversely to the general slope and overall drainage pattern. In the valleys alluvial soils have formed consisting of redeposited sand, loam and peat. Because of the intensive agricultural drainage of the areas, these peaty soils are strongly oxidized and have often become very thin. The majority of the area consists of cultivated land with grassland and maize being the most frequently occurring crops.

The soil data for the Beerze-Reusel basin was categorized into more than 12,000 influence areas (Wöster et al., 2001). In the database these are given as GIS polygons whose spatial arrangement is shown in Figure 5 at the top-right corner. In the RHSM each influence area is linked to a vertical column of 40 line elements of uniform size that discretize the generally about 2 m

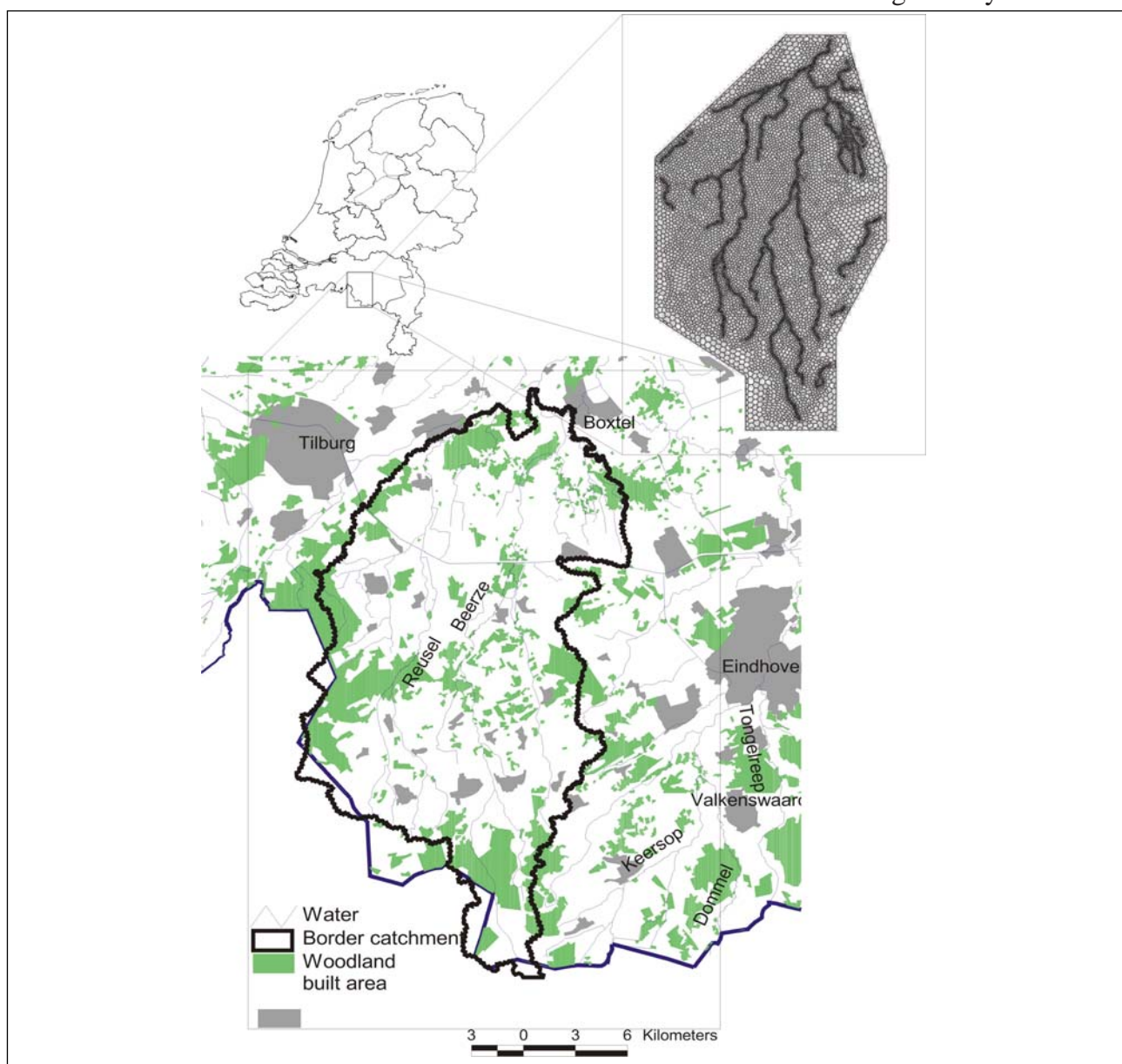


Figure 5. Map of the Meuse basin. Bottom inset shows the detailed map of the region. Top-right inset shows the influence area polygons.

thick soil layer. The database holds the SWCC for each soil type and their vertical arrangement through the model area. There are 56 distinct soil types discerned among the sand, loam and peat soils, which form 62 different soil profiles. The SWCC is pre-processed to describe the different soil properties specifically found in this basin. A complete description of all SWCC can also be found in Du et al. (2006).

Evaporation model

The RHSM simulation is driven by daily meteorological input data (precipitation, air temperature, sunshine duration) of the year 2000 in order to provide for a realistic system forcing. The raw time series data was taken from <http://eca.knmi.nl/dailydata/index.php>. From these data infiltration time series were calculated for the stations De Bilt, Twenthe, Vlissingen, Eindhoven, and Maastricht and transferred to the influence areas by inverse distance interpolation. By infiltration we refer to precipitation P_c minus potential evaporation E , if $P_c > E$, and zero infiltration otherwise. Figure 6 shows the precipitation amounts measured at Eindhoven over the year 2000 (top) and the corresponding calculated evaporation (bottom). It is important to note that it is the spatial variability of the infiltration series that makes every single local Richards problem unique in this study, i.e. even though only 62 distinct soil profiles exist, all roughly 12,000 local Richards problems have to be computed in order to achieve the correct regional representation of the Beerze-Reusel soil layer.

Potential evaporation, EMK , is computed by the Makkink method (Makkink, 1957), whose estimates are based on air temperature and the net shortwave radiation, R_s , only. Mathematically the Makkink estimate is defined as,

$$E_{MK} = C_{MK} \frac{1}{\lambda} \frac{R_s s}{s + \gamma} \tag{5}$$

where λ is the latent heat of water evaporation, γ is the psychrometric constant and s is the slope of saturated vapor pressure curve (a function of air temperature). The method assumes a constant ratio between net radiation and net shortwave radiation. The Makkink parameter, $CMK = 0.63$, was

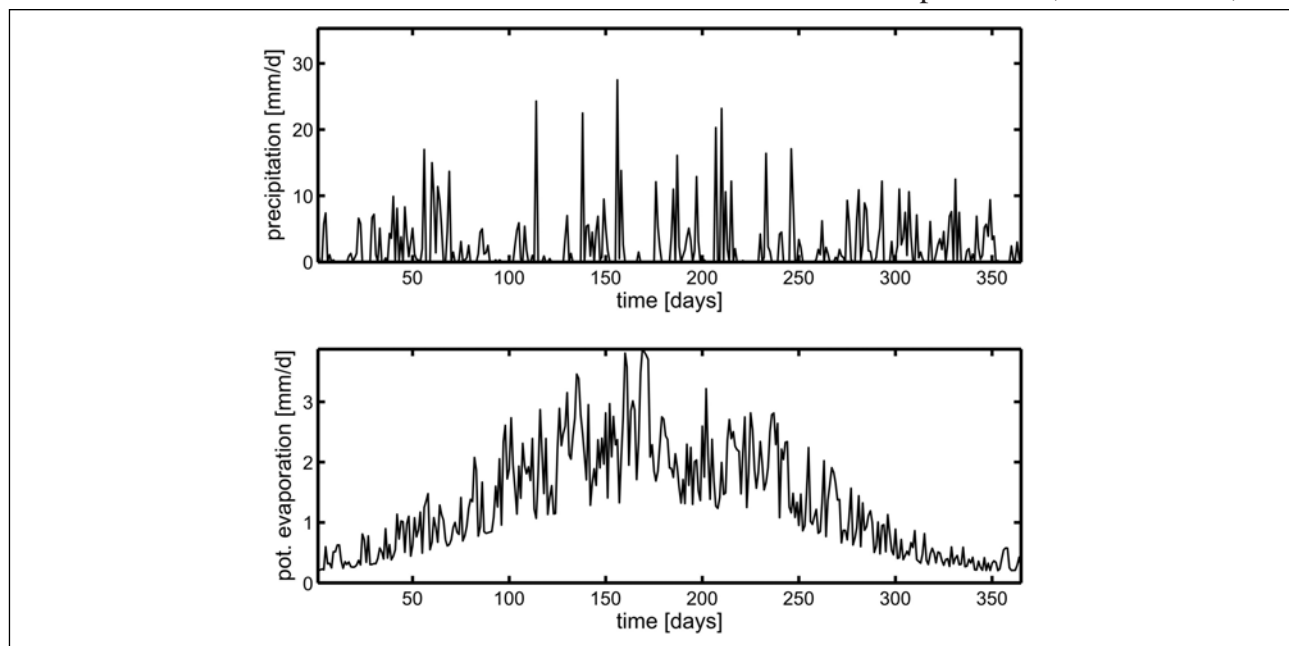


Figure 6. Precipitation and potential evaporation during the year 2000 for station Eindhoven.

chosen according to the findings of van Kraalingen and Stol (1997) for the Netherlands. Daily net shortwave radiation values are calculated based on the equations and recommendations given in Allen et al. (1998). A general albedo parameter of 0.23 is assumed, being representative of wet sand (Buttner and Sutter, 1935; Graser and Bavel, 1982) or dry grey soil (Kondrat'ev, 1954).

Simulation results

Single soil column

From the roughly 12,000 1D Richards problems two examples are shown below in Figure 7 together with their corresponding SWCC (i.e. capillary pressure- and relative permeability-saturation relationships). The top row of Figure 7 represents the functional behavior of a typical soil profile from the north of the basin, whereas the bottom row reflects the characteristics of the central region. Both soil profiles contain vertical changes of soil types (layered soil), hence, changing SWCC.

The simulation illustrates the difference in hydrologic response of both sites, which is mainly attributed to the soil heterogeneity in this case, rather than to the infiltration difference. Nevertheless, the parallelized RHSM provides a general means of computing spatially variable recharge patterns to groundwater created either by soil heterogeneity and/or the variation in water infiltration.

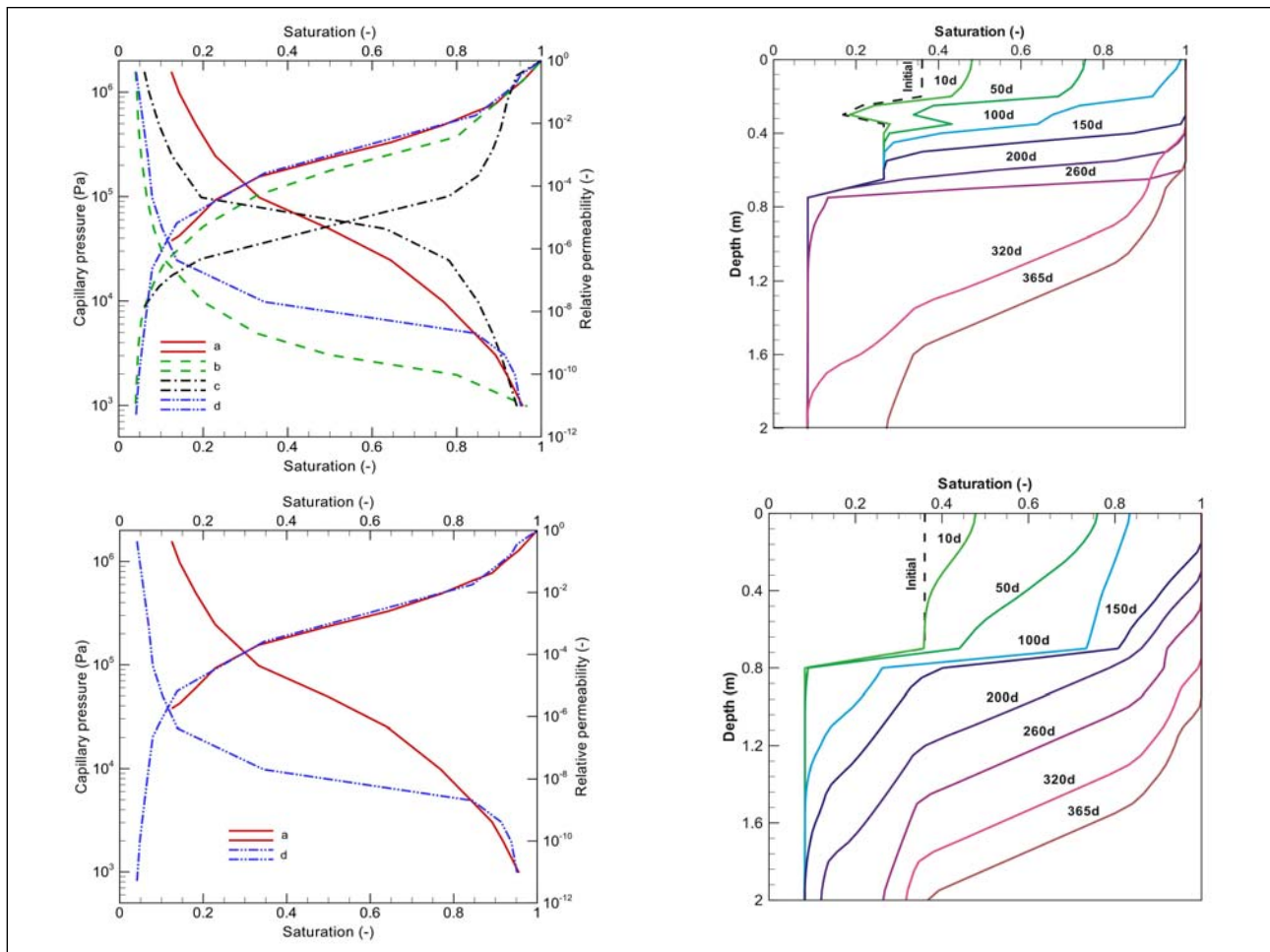


Figure 7. Soil water characteristic curves (SWCC) (left) and evolution of water saturation in selected soil columns (right). Top and bottom rows correspond to different sites of the basin. The time unit for the diagrams on the right is days [d].

Regional soil moisture patterns

The regional evolution of soil moisture patterns is shown in Figure 8 for day 30 and 60 of the year 2000. The influence of the lateral variation of soil profiles on the moisture transfer to the groundwater becomes quite evident, as the spatial variation of infiltration - even though existing - was found to be not so pronounced compared to the soil heterogeneity. Finally, the regional groundwater recharge distribution may be calculated from the bottom node soil water Darcy velocities, which were multiplied by the corresponding influence area for each soil profile.

Analysis of the computational performance

An important aspect of parallel computing is the efficient use of available computing resources. In this section we provide (parallel) computation times for an increasing number of processors and compare them to a serial run of the same problem size. Figure 9 depicts the graph of the functional relation between the measured computation time and the number of CPU's from one to eight and the resulting speed-up factors. It is important to note that the computation time includes also the data collection step at the end of each iteration.

A characteristic feature is that the speed-up factors level off, if more than four CPUs are used. This leveling off is believed to be due to the inherent broadcasting of results at the end of each parallel block. Even though all local Richards processes are set to the same model time period (one year) and number of time steps (366 days), the computation time for the solution of the individual non-linear Richards problems may vary. Considering that the Beerze-Reusel drainage basin consists of more than 12,000 influence areas and over 12,000 different transient boundary conditions, the estimation for the total computation time of individual Richards problems is not easily performed beforehand. This means that some processors may be idle while waiting for the

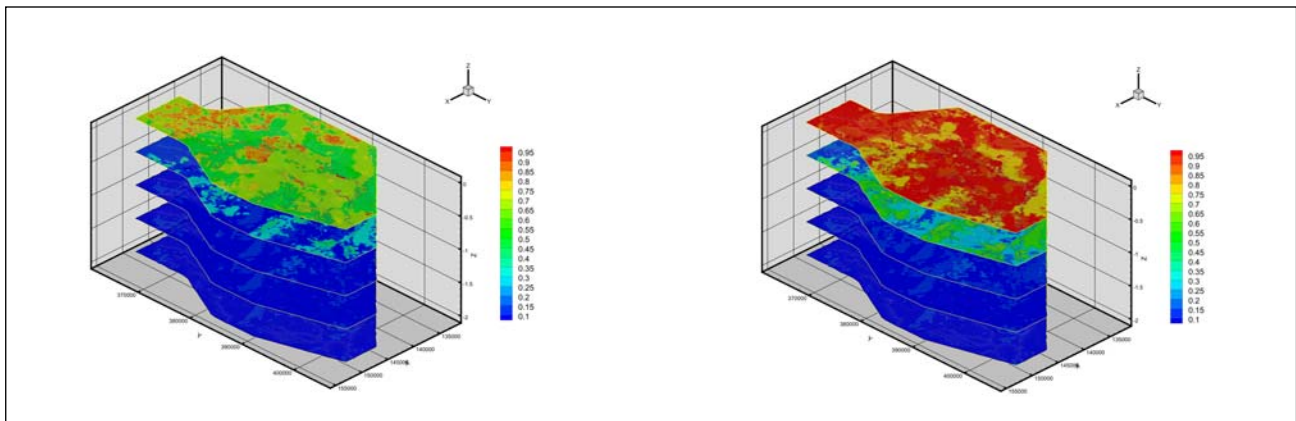


Figure 8. Regional water saturation distribution at days 30 and 60 (left and right, respectively).

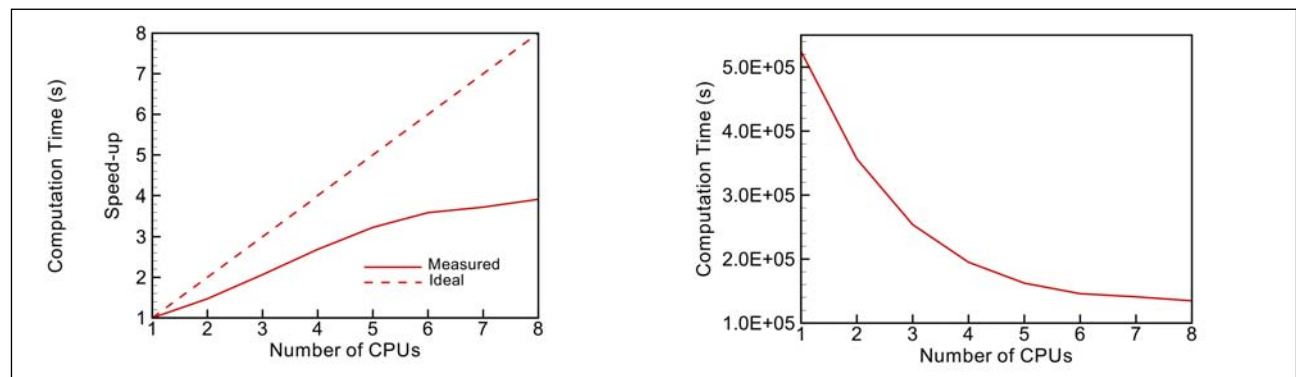


Figure 9. Execution times and resulting speed-up factors as a function of number of CPUs.

other processors to finish. As the parallel computation is only considered to be finished when results from all parallel processes are collected, it is this output aggregation that is believed to be the main cause of the reduction in computational performance. The key to optimize this parallel scheme could be the use of heuristic arguments (e.g. higher non-linearity of SWCC, higher heterogeneity of soil profiles, and higher expected computation times) to estimate computation times. Based on this estimation, the grouping of local Richards processes could be arranged in such a way that approximately the same computation time is necessary for each processor. Nevertheless, the optimal number of CPUs (i.e. four) for the parallel scheme used already reduced the computation time to almost 75% of the sequential (single processor) computation time.

SUMMARY AND CONCLUSIONS

The limitation of large-scale hydrological modeling stems from the requirement for small-scale discretization for accurate flow process representation on the one hand and the large areas to be covered on the other hand. Apart from the limitation in physical computer memory, it is the associated computation times that new computational approaches have to overcome. Within this framework, a RHSM combined with parallel computing techniques is proposed to tackle this problem. The key of the parallelized RHSM is to divide the massive computational demand into smaller computational units and achieve a parallel execution of these using the message passing interface. This study introduced the overall concept and the most important implementation details. A benchmark test showed the accuracy of the implementation by a direct comparison with MIN3P.

For a realistic test application, the Beerze-Reuzel drainage basin was selected for multi-scale hydrological modeling. Modeling this basin posed a challenge, as it covers an area of about 440 km² of heterogeneous soil with strong lateral variation. Using an evaporation model, as well as daily air temperature, precipitation, and sunshine duration data, infiltration series were calculated to provide a realistic meteorological forcing for the RHSM. Interestingly, the object-oriented programming framework of GS/RF also provided for a flexible integration of the RHSM and the evaporation model. Finally it was possible for the parallelized RHSM to compute the spatio-temporal evolution of soil moisture patterns for this large-scale within reasonable computation times. As a matter of fact, the computation time was reduced by 75% compared to a sequential run using four CPUs on a Linux cluster. The speed-up curve was found to be sub-critical indicating room for better optimization. Although this also demonstrates a limitation of the current approach, the proposed framework does provide a foundation for solving large-scale problems in hydrological systems.

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