THE IMPORTANCE OF THE UNSATURATED SOIL ZONE IN WATER ENGINEERING

Peter-Wolfgang Graeber

Okayama, March 27, 2013
Content of presentation

1. Processes in the unsaturated soil zone
2. Modelling of processes
3. Simulation tool PCSiWaPro®
4. Applications for PCSiWaPro®
   - Earth dams
   - Landfills
   - Seepage forecast
   - Small-scale wastewater treatment plants
   - Road drainage
   - Agriculture
1. Processes in the unsaturated zone

For the water cycle between atmosphere and groundwater the unsaturated soil zone plays an important role for the water balance as well as for the matter transport.
1. Processes in the unsaturated zone

Main focuses for consideration of water cycle:

- Agriculture (irrigation and drainage)
- Seepage forecast (water harvesting, treated sewage, pollution deposits, dumps, bank filtration, artificial groundwater recharge)
- Accompanied contaminant distribution in the soil
- Estimation of the stability of earth dams and dikes by analyzing the internal water saturation as flood protection
- Prognosis of stability of embankments / tilting of mines and traffic noise protection dams of roads and railways
- Calculation of groundwater recharge in dependence of soil parameters and precipitation scenarios
- Optimization of landfill covering systems
1. Processes in the unsaturated zone - Agriculture

Agriculture (irrigation, drainage) – problems:

- Salinization of agricultural areas
- Water-and nutrient balance of irrigated crops
- Contaminant comportment in irrigated soils
- Soils irrigated with treated wastewater effluents
- Influence of surface properties on runoff generation
- Land degradation problems and proposes to restoration soils

Irrigation is a fundamental requirement for agriculture in arid areas. The use of tools for modeling the unsaturated zone supports the sustainable management and control of water and soil resources.
1. Processes in the unsaturated zone – Water harvesting

Rain water harvesting to augment groundwater resources

Principle

- Rain water harvesting is the technique of collection and storage of rain water at surface or in sub-surface aquifers, before it is lost as surface run-off

- The augmented resource can be harvested in the time of need. Artificial recharge to ground water is a process by which the ground water reservoir is augmented at rate exceeding that under natural conditions of replenishment
1. Processes in the unsaturated zone – Water harvesting

Rain water harvesting to augment groundwater resources

Need
• To overcome the inadequacy of waters to meet our demands
• To arrest decline in groundwater levels
• To enhance availability of groundwater at specific place and time and utilize rain water for sustainable development
• To increase infiltration of rainfall water in the subsoil which has decreased drastically in urban areas due to paving of open area
• To improve groundwater quality by dilution
• To increase agriculture production
• To improve ecology of the area by increase in vegetation cover
1. Processes in the unsaturated zone – Water harvesting

Roof top rain water harvesting by recharge pit or trench
1. Processes in the unsaturated zone – Water harvesting

Model for groundwater harvesting (India)
1. Processes in the unsaturated zone – Dams and dikes

Instability of dams and dikes

Dike on river Danube

Dam in Syria
1. Processes in the unsaturated zone – Dams and dikes

Flood protection at a small river (Kaitzbach) in the surrounding of Dresden
1. Processes in the unsaturated zone – Dams and dikes

Flood on the river Weisseritz near of Dresden in 2002 (Background: Cotta-Bau (TU Dresden,)
Foto: H. Prasse
1. Processes in the unsaturated zone – Stability of slopes

Slope instability on the highway A 13 in the near of Dresden/Germany
1. Processes in the unsaturated zone – Stability in mines

Water balance in open-cast mining areas:

→ is an important tool for assessing the risk of landslides taking place at the peripheral slopes of the pit. Geo mechanical instabilities in a soil can already occur at a water saturation values below 100%.

An example about a landslide in a flooded lignite mine in Eastern Germany in 2010 is shown on the following pictures:
1. Processes in the unsaturated zone – Stability in mines
1. Processes in the unsaturated zone – Stability in mines
Processes in the unsaturated zone – Stability in minings
1. Processes in the unsaturated zone - Landfills

Optimization of landfill covering systems
1. Processes in the unsaturated zone - Landfills

Optimization of landfill covering systems
1. Processes in the unsaturated zone – Leachate forecast

Accompanied contaminant distribution in the soil

- Leachate
- Precipitation
- Contaminated site
- Place of assessment
- Unsaturated soil zone
- Capillary fringe
- Groundwater

groundwater table
1. Processes in the unsaturated zone – Leachate forecast

Assessment of groundwater vulnerability in the context of licensing procedures / regulations:

- Construction, waste, pollution, debris, road construction, backfilling (mines, quarries, gravel pits)
- Pesticides (herbicides, fungicides, insecticides, acaricides, nematicides, molluscicides, Rotentizide, Pyrethoide)
- Wood preservation agents (impregnating, ....)
- Binder (formaldehyde, etc.)
- Roading salt
1. Processes in the unsaturated zone – Leachate forecast

Soil contamination

Which parameters influence contaminant transport in the unsaturated zone of the soil the most?

Example:
- Tank farm, used for a long time
- Massive groundwater contamination with BTEX

Arising questions:
- Highest BTEX concentration in leachate?
- Time span reaching the groundwater zone?
- Total BTEX mass entering the groundwater zone?
1. Processes in the unsaturated soil zone

2. Modelling of processes

3. Simulation tool PCSiWaPro®

4. Applications for PCSiWaPro®
   - Earth dams
   - Landfills
   - Seepage forecast
   - Road drainage
   - Small-scale wastewater treatment plants
   - Agriculture
2. Modelling for the unsaturated zone
2. Modelling for the unsaturated zone

**Why** modelling?

- faster, less expensive than field experiments
- risk assessment, prognosis
- scenario analysis (best case/worst case, ...)
- process understanding

**But**: The more processes included in a model, the more difficult parameterization becomes!

- water flow, root water uptake, plant growth, preferential flow, contaminant transport, sorption, decay, chemical reactions, soil-surface-interaction, soil-groundwater-interaction, ...
2. Modelling for the unsaturated zone

Source: Hölting (1996)
2. Modelling for the unsaturated zone

The unsaturated soil zone plays an important role for the transport of surface water into the ground water as well as for the matter transport. This processes can predicted by models.

For modelling of this processes can be used

• physical models (channels, columns, lysimeters, ) and/or

• mathematical models
  Water flow acc. to RICHARDS-equation,
  soil hydraulics acc. to VAN GENUCHTEN-LUCKNER
  Transport modeling: advection dispersion equation
2. Modelling for the unsaturated zone

Background of mathematical models:

- **RICHARDS- Equation** → flux and water balance

\[
\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i} \left[ K \left( K_{ij}^A \frac{\partial h}{\partial x_j} + K_{iz}^A \right) \right] - S
\]

- Parameterization of soil characteristics by VAN GENUCHTEN-LUCKNER (Water retention curve)

\[
\theta = \theta_r + \frac{\phi - \theta_{r,w} - \theta_{r,l}}{\left[ 1 + (\alpha \cdot h_c)^n \right]^{1/n}}
\]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\theta)</td>
<td>volumetric water content</td>
</tr>
<tr>
<td>(t)</td>
<td>time</td>
</tr>
<tr>
<td>(x_i)</td>
<td>((x_1=x, x_2=z)), spatial coordinates</td>
</tr>
<tr>
<td>(K)</td>
<td>hydraulic conductivity</td>
</tr>
<tr>
<td>(h)</td>
<td>pressure head</td>
</tr>
<tr>
<td>(S)</td>
<td>sink/source term</td>
</tr>
<tr>
<td>(\phi)</td>
<td>porosity</td>
</tr>
<tr>
<td>(\theta_{r,w})</td>
<td>residual water content</td>
</tr>
<tr>
<td>(\theta_{r,l})</td>
<td>residual air content</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>scaling factor (van Genuchten)</td>
</tr>
<tr>
<td>(n)</td>
<td>slope factor (van Genuchten)</td>
</tr>
<tr>
<td>(h_c)</td>
<td>capillary pressure head</td>
</tr>
</tbody>
</table>
2. Modelling for the unsaturated zone

Retention curve

2. Modelling for the unsaturated zone

Retention curve (water content – capillary pressure)

- Porosity \( \phi = 0.36 \)
- Residual non-wetting fluid content \( B_\text{r} = 0.144 \)
- Residual wetting fluid content \( A_\text{r} = 0.113 \)

- PDC - Primary Drainage Curve
- SWC - Scanning Wetting Curve
- SDC - Scanning Drainage Curve
- MWC - Main Wetting Curve
- MDC - Main Drainage Curve
2. Modelling for the unsaturated zone

Relative unsaturated hydraulic permeability

- $S_0 = 1.0$
- $S_0 = 0.86$
2. Modelling for the unsaturated zone

\[ \frac{\partial c}{\partial t} + \frac{\partial ps}{\partial t} = \frac{\partial}{\partial x_i} \left( \theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s ps + \gamma_w \theta + \gamma_s \rho - Sc_s \]

- \( c \): concentration
- \( s \): sorbed concentration
- \( \rho \): bulk density
- \( t \): time
- \( q_i \): \( i \)-th component of flux
- \( \theta \): water content
- \( D_{ij} \): tensor of dispersion coefficients
- \( S \): sink/source term
- \( C_s \): concentration of sink/source term
- \( \gamma \): parameters for 0\textsuperscript{th} order processes
- \( \mu \): parameters for 1\textsuperscript{st} order processes

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>( D_{ij}, S, C_s )</th>
<th>( Y_w, Y_s, \mu_w, \mu_s )</th>
</tr>
</thead>
<tbody>
<tr>
<td>c</td>
<td>concentration</td>
<td></td>
<td></td>
</tr>
<tr>
<td>s</td>
<td>sorbed concentration</td>
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<td>( t )</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>( q_i )</td>
<td>( i )-th component of flux</td>
<td></td>
<td></td>
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</table>
2. Modelling for the unsaturated zone

→ Models described by **partial differential equations**:

→ **Transport**: Convection-Dispersion-Equation

\[
\frac{\partial \theta c}{\partial t} + \frac{\partial \rho s}{\partial x} = \frac{\partial}{\partial x_i} \left( \theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - Sc_s
\]

sorption

→ attachment and detachment of contaminants to **soil body**

→ described by **isotherms**
2. Modelling for the unsaturated zone

→ **Sorption isotherms**

→ **HENRY**: linear, for low concentrations

\[ S_m = \theta \cdot \rho_{fl,m} + \rho_b \cdot K_d \cdot \rho_{fl,m} = (\theta + \rho_b K_d) \rho_{fl,m} \]

→ **FREUNDLICH**: exponential, for fixed number of sorption spots

\[ S_m = \theta \cdot \rho_{fl,m} + K_F \cdot \rho_{fl,m}^q \]

→ **LANGMUIR**: non-linear, for high-concentrations

\[ S_m = \theta \cdot \rho_{fl,m} + \frac{K_L \cdot \rho_{fl,m}}{1 + K_L \cdot \rho_{fl,m}} \cdot S_{s,\text{max}} \]

\( s_m \) – adsorbed mass on the solid phase
\( \theta \) – water content, \( \rho_b \) – soil bulk density, \( \rho_{fl,m} \) – partial mass density in the fluid phase
\( K_d \) – partitioning-(HENRY)-coefficient, \( q \) – constant parameter, \( K_F \) – FREUNDLICH-coefficient
\( S_{s,\text{max}} \) – max. adsorbed mass on the solid phase, \( K_L \) – LANGMUIR-coefficient
2. Modelling for the unsaturated zone

→ Models described by **partial differential equations:**

→ **Transport:** Convection-Dispersion-Equation

\[
\frac{\partial \theta c}{\partial \tilde{t}} + \frac{\partial \rho s}{\partial \tilde{t}} = \frac{\partial}{\partial \tilde{x}_i} \left( \theta D_{ij} \frac{\partial c}{\partial \tilde{x}_j} \right) - \frac{\partial q_i c}{\partial \tilde{x}_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - Sc_s
\]

**dispersion/diffusion**

→ dispersion coupled to **convection**

→ diffusion due to **Brownian** movement
2. Modelling for the unsaturated zone

→ Models described by **partial differential equations:**

→ **Transport**: Convection-Dispersion-Equation

$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho s}{\partial t} = \frac{\partial}{\partial x_i} \left( \theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - Sc_s$$

**convection**

→ transport with the **flow of water**
2. Modelling for the unsaturated zone

→ Models described by **partial differential equations:**

→ **Transport:** Convection-Dispersion-Equation

\[
\frac{\partial \theta c}{\partial t} + \frac{\partial s \rho}{\partial x} = \frac{\partial}{\partial x_i} \left( \theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - Sc_s
\]

0th/1st order internal reactions

→ **internal** production or degradation

\[
\frac{ds_m}{dt} = -\mu_m \cdot s_m
\]

→ **example:** exponential **decay**

\[
s_m = s_{m,0} \cdot e^{-\mu_m \cdot t}
\]
2. Modelling for the unsaturated zone

→ Models described by **partial differential equations:**

**Transport:** Convection-Dispersion-Equation

\[
\frac{\partial \theta c}{\partial t} + \frac{\partial \rho s}{\partial x} = \frac{\partial}{\partial x_i} \left( \theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - Sc_s
\]

→ contaminant concentration at model **boundary**

→ **source term** functions
2. Modelling for the unsaturated zone

How to use these equations to **simulate** model behaviour

- **input data**
  - soil parameters (conductivities, porosities, ...)
  - contaminant parameters (diffusion coefficient, half-life, ...)
  - initial conditions
  - steady-state or transient **boundary** conditions

- mathematical equation **solving technique**
  - additional input data: **discretization** of the model area (space and time)
1. Processes in the unsaturated soil zone

2. Modelling of processes

3. **Simulation tool PCSiWaPro®**

4. Applications for PCSiWaPro®
   - Earth dams
   - Landfills
   - Seepage forecast
   - Road drainage
   - Small-scale wastewater treatment plants
   - Agriculture
3. Simulation tool PCSiWaPro®

PCSiWaPro®

- 2D-simulation of steady-state/transient water balance and transport processes in unsaturated zone
- easy to handle Windows Software
- GUI that is adapted to several languages (German, English, Spanish, French, Polish, Japanese, Vietnamese, Arabic)
- easy presentation of the results due to several interfaces to graphical software
- flexible choice of boundary conditions
- consideration of atmospheric boundary conditions, root water uptake and soil evaporation; contaminant degradation, sorption
- consideration of hysteretic processes within the unsaturated zone
- implemented algorithm for parameter identification
- integrated weather generator for arbitrary time series in high resolution
- automatic discretization with Galerkin finite element mesh generator
- soil databases DIN 4022, DIN 4220, UNSODA, RESETA, pedotransfer function
3. Simulation tool PCSiWaPro®

→ **PCSiWaPro®**: a software to *simulate* flow and transport processes in the unsaturated soil zone

(1) model **generator**

(2) system **solver**

(3) result **viewer**
3. Simulation tool PCSiWaPro®

How to use these equations to simulate model behaviour with PCSiWaPro®

- **input data**
  - *soil* parameters (conductivities, porosities, ...)
  - *contaminant* parameters (diffusion coefficient, half-life, ...)
  - **initial** conditions
  - steady-state or transient **boundary** conditions

- mathematical equation **solving technique**
  - additional input data: **discretization** of the model area (space and time)
Integrated 1D- or 2D-mesh generator
3. Simulation tool PCSiWaPro®

➔ How to use these equations to simulate model behaviour with PCSiWaPro®

➔ **input data**
  ➔ **soil** parameters (conductivities, porosities, ...)
  ➔ **contaminant** parameters (diffusion coefficient, half-life, ...)
  ➔ **initial** conditions
  ➔ steady-state or transient **boundary** conditions

➔ mathematical equation **solving technique**
  ➔ additional input data: **discretization** of the model area (space and time)
3. Simulation tool PCSiWaPro®

→ Data input through user-friendly GUI

→ **input data** from:
  1. integrated databases
  2. pedotransfer functions
  3. measured data

→ **selection of model assumptions**
  → sorption isotherms
  → source term functions
How to use these equations to simulate model behaviour with PCSiWaPro®

- input data
  - soil parameters (conductivities, porosities, ...)
  - contaminant parameters (diffusion coefficient, half-life, ...)
  - initial conditions
  - steady-state or transient boundary conditions

- mathematical equation solving technique
  - additional input data: discretization of the model area (space and time)
3. Simulation tool PCSiWaPro®

Equations solved by:

- **discretization**
  - space: **finite elements**
  - time: adjusted **finite intervals**
    - explicit, implicit, Crank-Nicholson

- repeated solution of **linear equation system** for each timestep
  - **direct**: Gaussian elimination
  - **iterative**: preconditioned conjugate gradient method

- **Problem**: long simulation runtimes
3. Simulation tool PCSiWaPro®

Acceleration by **Parallelization**!

- 2 ways: automatically (Compiler, Hardware) *manually* (Code)

- Only for **independent** code parts
  - possible: 
    ```
    do i = 1, 20000
        a(i) = 3*i + 16
    end do
    ```
  - not possible: parallel calculation of different time steps of a simulation

- Basic concept: **partitioning & synchronization** of work & data
3. Simulation tool PCSiWaPro®

→ Concept 1: **OpenMP** (Open Multi-Processing)

→ Partitioning of **loop iterations** (as seen before)
→ several „threads“ access **shared** memory
→ „incremental“ parallelization
→ **feasible** for \( \leq 8 \) processor cores
3. Simulation tool PCSiWaPro®

Concept 2: **MPI** (Message Passing Interface)

- Partitioning of **work** and **data**
- several „**processes**“ with private memory work independently and communicate via „messages“
- **Distributed**-Memory
- „**full**“ parallelization
- theoretically **scalable** for any number of processors (→ Amdahl's law)
Amdahl's law

\[ T(p) \ldots \text{runtime of a program with } p \text{ processes/threads} \]
\[ s \ldots \text{not parallelizable part of the program } (0 < s < 1) \]
\[ S(p) \ldots \text{acceleration factor with } p \text{ processes/threads ("speedup")} \]

\[ S(p) = \frac{T(1)}{T(p)} = \frac{1}{s + \frac{1-s}{p}} \]

(1) \( s=0 \rightarrow S(p) = p \)
(2) \( p=\infty \rightarrow S(p) = \frac{1}{s} \)
3. Simulation tool PCSiWaPro®

- individual **challenges**

  - OpenMP: **rewriting** loops for parallelization  
    - not always possible

  - MPI: **communication** at internal boundaries

- computationally most **expensive** tasks:
  1. matrix assembly
  2. system solver

- testing of **parallel solver libraries**
Parallelization of sequential PCSiWaPro® using MPI

Launch of PCSiWaPro® with several processes

User interaction only with process 0 (P0)
- other processes in waiting loop
- called by P0 for selected code parts

PCSiWaPro® written in VB.NET and FORTRAN
- MS-MPI to execute MPI commands
- MPI.NET to call MPI functions from .NET environment
3. Simulation tool PCSiWaPro®

→ (A) flow and transport matrix assembly

→ initially node data only available for P0

→ 2 possibilities:
  (1) assembly of A by P0, then distribution
  (2) distribution of node data, then assembly
  of submatrices by each process

→ parallel overhead smaller for (1) than for (2)
→ one-time distribution of submatrices
→ no communication needed during matrix assembly
3. Simulation tool PCSiWaPro®

→ **Direct** equation solvers

→ **Libraries**
  → OpenMP: Pardiso (Intel Math Kernel Library)
  → MPI: MUMPS (Université de Toulouse, ENS Lyon)

→ **Steps:**
  (1) matrix factorization (LU, Cholesky, ...)
    → very **expensive**!
  (2) system solving

\[
\begin{align*}
\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 10 \end{pmatrix}
&= 
\begin{pmatrix} 1 & 0 & 0 \\ 4 & 1 & 0 \\ 7 & 2 & 1 \end{pmatrix}
\begin{pmatrix} 1 & 2 & 3 \\ 0 & -3 & -6 \\ 0 & 0 & 1 \end{pmatrix}

A \cdot x &= L \cdot U \cdot x = B \\
L \cdot (U \cdot x) &= L \cdot y = B \quad \rightarrow y \\
A &= L \cdot U \\
U \cdot x &= y \quad \rightarrow x
\end{align*}
\]
3. Simulation tool PCSiWaPro®

→ **Iterative** equation solvers

→ **Libraries** with several iterative solvers and preconditioners
  - MPI: **PETSc** (Argonne National Laboratory)
  - MPI: **Lis** (Japan Science and Technology Agency)

<table>
<thead>
<tr>
<th></th>
<th>PETSc</th>
<th>Lis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data distribution</td>
<td>automatically</td>
<td>manually</td>
</tr>
<tr>
<td>Flow</td>
<td>CG, Jacobi</td>
<td>GMRES, I+S</td>
</tr>
<tr>
<td>Transport</td>
<td>BiCGSTAB, Jacobi</td>
<td>BiCG, ILU</td>
</tr>
</tbody>
</table>

\[ r = A \cdot x - B \]
\[ \text{precon}(A) \]
\[ \text{while}(\text{norm}(r) > \text{tol}) \]
\[ \text{calculate}(x) \]
\[ r = A \cdot x - B \]
3. Simulation tool PCSiWaPro®

→ (B) system solver: parallel **iterative** equation solver libraries

→ manual data distribution with **Lis**

<table>
<thead>
<tr>
<th>Matrix:</th>
<th>10</th>
<th>9</th>
<th>0</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>7</td>
<td>0</td>
<td>0</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>0</td>
<td>5</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>2</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

**CRS format:** values = \( (10,9,8,7,6,5,4,3,2,1) \)
columns = \( (0,1,3,0,3,2,3,0,1,3) \)
rows = \( (0,3,5,7,10) \)

→ **row-wise** distribution on processes
→ simple example: 4 rows, 4 processes, 1 row per process
3. Simulation tool PCSiWaPro®

→ (B) system solver: parallel **iterative** equation solver libraries

→ manual data distribution with **Lis**: creation of CRS arrays from original storage format

(1) **OpenMP-parallel** calculation of values/columns arrays

→ calculation of **NNZ** for each process

→ **starting position** for threads to write in the values/columns arrays

<table>
<thead>
<tr>
<th>P0</th>
<th>P1</th>
<th>P2</th>
<th>P3</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>values</strong></td>
<td>(10, 9, 8)</td>
<td>7, 6,</td>
<td>5, 4,</td>
</tr>
<tr>
<td><strong>columns</strong></td>
<td>(0, 1, 3,</td>
<td>0, 3,</td>
<td>2, 3,</td>
</tr>
</tbody>
</table>
3. Simulation tool PCSiWaPro®

→ (B) system solver: parallel **iterative** equation solver libraries

→ manual data distribution with **Lis**: creation of CRS arrays from original storage format

(2) **OpenMP-parallel** calculation of **rows** array

→ **original** storage format (different matrix here):

\[
\text{rows\_old} = (3,2|2,1|1,3|4,2)
\]

→ parallel **summation**: (3,5|2,3|1,4|4,6)

→ summation of **NNZ** of each process: \((0,5,8,12,18)\)

→ final parallel construction of complete **rows**:

\[
(0,3+0,5+0|2+5,3+5|1+8,4+8|4+12,6+12)
\]

\[
= (0,3,5|7,8|9,12|16,18)
\]
3. Simulation tool PCSiWaPro®

- (B) system solver: parallel **iterative** equation solver libraries

- manual data distribution with **Lis:** **distribution** of CRS arrays from P0 to other processes

<table>
<thead>
<tr>
<th></th>
<th>Total</th>
<th>P0</th>
<th>P1</th>
<th>P2</th>
<th>P3</th>
</tr>
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<tbody>
<tr>
<td>values</td>
<td>(10,9,8,7,6,5,4,3,2,1)</td>
<td>(10,9,8)</td>
<td>(7,6)</td>
<td>(5,4)</td>
<td>(3,2,1)</td>
</tr>
<tr>
<td>columns</td>
<td>(0,1,3,0,3,2,3,0,1,3)</td>
<td>(0,1,3)</td>
<td>(0,3)</td>
<td>(2,3)</td>
<td>(0,1,3)</td>
</tr>
<tr>
<td>rows</td>
<td>(0,3,5,7,10)</td>
<td>(0,3)</td>
<td>(0,2)</td>
<td>(0,2)</td>
<td>(0,3)</td>
</tr>
</tbody>
</table>

- **values/columns:** subarrays by **dividing** original array
- **rows:** subarrays by **recalculation**
- **or:** easier by using **rows_old**:
  \[(3,2|2,1|1,3|4,2) \rightarrow (0,3,5) (0,2,3) (0,1,4) (0,4,6)\]
3. Simulation tool PCSiWaPro®

- **Runtimes** for Lis, PETSc, sequential
  (4 processes, Intel Xeon 3470, 2.93 GHz, 8GB RAM)

<table>
<thead>
<tr>
<th></th>
<th>Model 1</th>
<th>Model 2</th>
<th>Model 3</th>
<th>Model 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nodes</td>
<td>952</td>
<td>1.436</td>
<td>18.531</td>
<td>135.019</td>
</tr>
<tr>
<td>Nonzero</td>
<td>6.164</td>
<td>18.626</td>
<td>127.911</td>
<td>942.081</td>
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</table>

<table>
<thead>
<tr>
<th></th>
<th>Lis</th>
<th>PETSc</th>
<th>sequential</th>
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<tbody>
<tr>
<td></td>
<td>29.0s</td>
<td>27.8s</td>
<td>11.6s</td>
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<tr>
<td></td>
<td>17.4s</td>
<td>16.7s</td>
<td>5.5s</td>
</tr>
<tr>
<td></td>
<td>4m58s</td>
<td>4m29s</td>
<td>1m33s</td>
</tr>
<tr>
<td></td>
<td>7h34m01s</td>
<td>3h26m56s</td>
<td>3h40m35s</td>
</tr>
</tbody>
</table>

The simulation software PCSiWaPro®
3. Simulation tool PCSiWaPro®

→ Result: MPI not feasible

   (1) number of nodes
   (2) software type
   (3) machine type

→ alternative: multigrid solver SAMG

→ Fraunhofer-Institute
→ excellent convergence
→ cheap coarse direct solver
→ parallelized with OpenMP
### Runtimes for SAMG

(4 threads, Intel Xeon 3470, 2.93 GHz, 8GB RAM)

<table>
<thead>
<tr>
<th></th>
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<th>Model 3</th>
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</tr>
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<td>942.081</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>SAMG</th>
<th>sequential</th>
<th></th>
<th></th>
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<tbody>
<tr>
<td></td>
<td>16,1s</td>
<td>6,0s</td>
<td>1m15s</td>
<td>0h22m21s</td>
</tr>
<tr>
<td></td>
<td>-39%</td>
<td>-9%</td>
<td>+19%</td>
<td>+89%</td>
</tr>
</tbody>
</table>

3. Simulation tool PCSiWaPro®
3. Simulation tool PCSiWaPro®

**Runtimes for SAMG**

(4 threads, Intel Xeon 3470, 2.93 GHz, 8GB RAM)

<table>
<thead>
<tr>
<th></th>
<th>Model 5</th>
<th>Model 6</th>
<th>Model 7</th>
<th>Model 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nodes</td>
<td>3.138</td>
<td>8.689</td>
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<td>21.221</td>
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<tr>
<td>Nonzero</td>
<td>21.402</td>
<td>60.382</td>
<td>127.911</td>
<td>147.221</td>
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</table>

<table>
<thead>
<tr>
<th></th>
<th>1m36s</th>
<th>1m15s</th>
<th>1m28s</th>
<th>2m25s</th>
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<tbody>
<tr>
<td>SAMG</td>
<td>sequential</td>
<td>percentage</td>
<td>sequential</td>
<td>percentage</td>
</tr>
<tr>
<td></td>
<td>1m53s</td>
<td>+15</td>
<td>1m34s</td>
<td>+20</td>
</tr>
<tr>
<td></td>
<td>2m09s</td>
<td>+32</td>
<td>12m21s</td>
<td>+81</td>
</tr>
</tbody>
</table>
Conclusion of Parallelisation

1. PCSiWaPro® is a tool for modeling unsaturated zone processes.

2. The tasks that needed acceleration were the assembly of the coefficient matrices and the solving of the linear equation systems.

3. Due to the software type of PCSiWaPro and the usual mesh sizes, MPI parallelization was not the feasible option for acceleration.

4. OpenMP was used to parallelize big loops in the matrix assemblies.

5. The solver finally implemented is based on OpenMP-parallelized multigrid methods.
3. Simulation tool PCSiWaPro® - WettGen

How to use these equations to simulate model behaviour with PCSiWaPro®

- **input data**
  - **soil** parameters (conductivities, porosities, ...)
  - **contaminant** parameters (diffusion coefficient, half-life, ...)
  - **initial** conditions
  - steady-state or transient **boundary** conditions

- mathematical equation **solving technique**
  - additional input data: **discretization** of the model area
    (space and time)
3. Simulation tool PCSiWaPro® - WettGen

→ Computation of upper boundary condition with the integrated *weather generator*

→ **input** data
  → precipitation
  → evapotranspiration
  → vegetation cover
  → slope
  → …

→ **output**: daily values of precipitation
3. Simulation tool PCSiWaPro® - WettGen

⇒ **Time series generation** by:

(1) statistical **characterization** of input time series
(2) spatial **interpolation** of statistical parameters
(3) **sampling** of synthetical time series
⇒ past, present and **future**
3. Simulation tool PCSiWaPro® - WettGen

Data input through assistant
3. Simulation tool PCSiWaPro® - WettGen

- Graphical visualization of result **time series**
- **automatic transfer** to PCSiWaPro® model
Motivation

- pure consideration of **fully saturated** for simulating the water balance in mining areas disregards:
  - different **weather** conditions
  - saturation effects in **partially saturated** soil

- **groundwater recharge** in GW model not static, but result of unsaturated soil zone simulation
- **coupling** of simulation of both soil zones

- **Effects** on GW table dynamics, pit slope stability, ...
Coupling of PCGeofim® and PCSiWaPro®

→ **PCSiWaPro®**: software for unsaturated soil zone simulation

→ 2D simulation of **water flow** and **contaminant transport**
   → Van Genuchten / Luckner **soil model** including hysteresis

→ integrated mesh generator for numerical **finite element** discretization

→ flexible **boundary conditions**: prescribed groundwater tables / pressure heads, atmospheric BCs, root water uptake, evaporation, ...

→ integrated weather generator **WettGenWH** for daily values of atmospheric time series

→ soil data **sources**: integrated databases (DIN 4022, DIN 4220) pedotransfer functions
Coupling of PCGeofim® and PCSiWaPro®

→ **PCGeofim®**: software for groundwater flow and transport simulation in *mining* regions

→ simulation in **3D** and **2D** (intersections)

→ **horizontal** finite volumes discretization

→ **transport** modeling by:
  (1) PHREEQC coupling
  (2) Random-Walk-method

→ **static** groundwater recharge modeling
## Coupling challenges

<table>
<thead>
<tr>
<th>Modeling</th>
<th>Software</th>
<th>Simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>interface <strong>description</strong></td>
<td>software communication <strong>design</strong></td>
<td>interaction <strong>sequence</strong></td>
</tr>
<tr>
<td>transfer parameter <strong>definition</strong></td>
<td>transfer data format <strong>selection</strong></td>
<td>Discretization <strong>mapping</strong></td>
</tr>
<tr>
<td></td>
<td>simulation code <strong>modification</strong></td>
<td></td>
</tr>
</tbody>
</table>
Coupling of PCGeofim® and PCSiWaPro®

- **Coupling type:** PCSiWaPro® (2D) with PCGeofim®-intersections

- **real interface:** GW table as place of **GW recharge**

- both models cover the **whole** area, in which the GW table **can** lie during the simulation

- 3 **transfer parameters** ...
Coupling of PCGeofim® and PCSiWaPro®

→ **Transfer parameters** of the coupling

→ **GW recharge rate**
  → calculated by PCSiWaPro® using *internal fluxes*
  at the nodes of the current GW table
  → Transfer to PCGeofim® as **upper boundary condition**
Coupling of PCGeofim® and PCSiWaPro®

→ Transfer parameters of the coupling

→ GW recharge rate
  → calculated by PCSiWaPro® using internal fluxes at the nodes of the vurrent GW table
  → Transfer to PCGeofim® as upper boundary condition

→ vertical GW table position
  → Transfer from PCGeofim® to PCSiWaPro®
    → adjustment of the current saturation values
Coupling of PCGeofim® and PCSiWaPro®

→ **Transfer parameters** of the coupling

→ **GW recharge rate**
  - calculated by PCSiWaPro® using *internal fluxes*
  - at the nodes of the current GW table
  - Transfer to PCGeofim® as *upper boundary condition*

→ **vertical** GW table position
  - Transfer from PCGeofim® to PCSiWaPro®
  - **adjustment** of the current saturation values

→ **horizontal** positions of the discretization units
  (Mapping PCSiWaPro® *nodes* to PCGeofim® *volumes*)
Coupling of PCGeofim® and PCSiWaPro®

- Calculation of internal fluxes in PCSiWaPro® model:
  (0) initial mesh
Coupling of PCGeofim® and PCSiWaPro®

→ Calculation of internal fluxes in PCSiWaPro® model:
(1) calculation of nodal fluxes
Coupling of PCGeofim® and PCSiWaPro®

→ Calculation of internal fluxes in PCSiWaPro® model:
  (2) calculation of nodal fluxes at the GW table
Coupling of PCGeofim® and PCSiWaPro®

→ Calculation of internal fluxes in PCSiWaPro® model:

(3) calculation of edge fluxes at the GW table
Coupling of PCGeofim® and PCSiWaPro®

→ Calculation of internal fluxes in PCSiWaPro® model:

(4) mapping of edge fluxes to PCGeofim® volumes
Coupling of PCGeofim® and PCSiWaPro®

→ test model for validation

→ 5m column with fine sand

→ simulation for 730d

→ 440mm precipitation in first 365d
Coupling of PCGeofim® and PCSiWaPro®

→ GW recharge for different GW table depths
Coupling of PCGeofim® and PCSiWaPro®

⇒ lysimeter experiment for validation

⇒ 3m columns with undisturbed podsol

⇒ locally measured precipitation and evapotranspiration, and root water uptake by winter wheat as upper boundary condition

⇒ Water saturation measurements initial condition

⇒ Outflow at the soil bottom as comparative for calculated GW recharge

Coupling of PCGeofim® and PCSiWaPro®

- lysimeter experiment for validation
Coupling of PCGeofim® and PCSiWaPro®

→ GW table **adjustment** in PCSiWaPro®

→ **rise**: set \( h \) in the GW area  
→ **drop**: additional interpolation above the GW table

→ **manual** adjustment of the GW table in PCSiWaPro® interpreted as **artificial**  
water influx/outflux

→ **correction** of the internal water balance by comparing **model water amount**  
before and after the adjustment

→ “**influx**” calculated via \( \theta(t_1) - \theta(t_0) \)
**Coupling of PCGeofim® and PCSiWaPro®**

→ *Interaction sequence*: **parallel** (online coupling)

→ models must **data exchange times** exactly
  → common realization of an **exchange timetable**

→ Comparison to sequential coupling (offline):
  → **pro**: better modelling accuracy
  → **contra**: higher probability of numerical instabilities (different model scales, ...)

![Diagram of model coupling](image.png)
Future work

**Implementation** of boundary condition transfer in PCGeofim®

- technical **design** of *software communication*:
  - *interfaces* for **data exchange** during the simulation
    (ASCII/binary files, shared memory)
  - **criteria**: stability, time expenditure

- common **data storage** after the simulation
  - MS Access, HDF5
  - complete project data, time series of exchanged
    boundary conditions
Thank you for your attention

»Wissen schafft Brücken.«

>> Knowledge builds bridges <<