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JÜLICH FORSCHUNGSZENTRUM

Investigation of Grid-partioning for parallel modelling of root water uptake

18. Oktober 2010 | Martin Licht

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Joint project of JSC and ICG IV

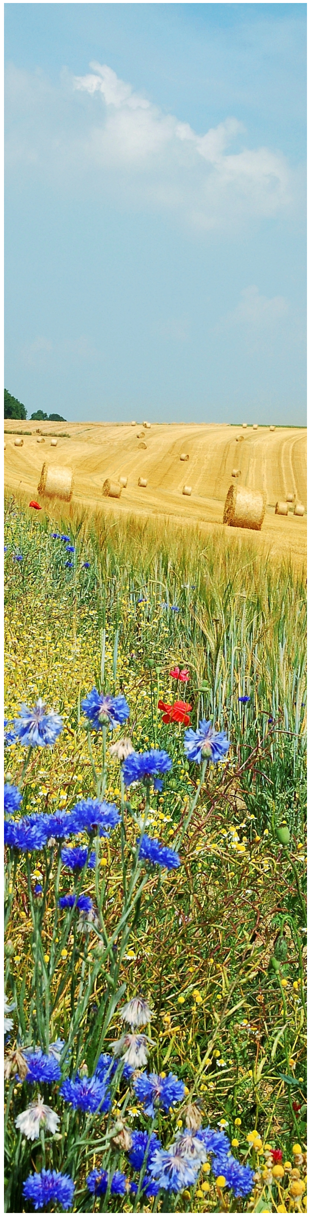
JSC Guest student program 2010

Agenda

- **Part 1 : Introduction**
- Part 2 : Numerical Model
- Part 3 : Software implementation
- Part 4 : Parallizing Root water uptake
- Part 5 : Conclusions

Context

- Plants are a vast domain of life and of tremendous importance for human culture
- Yet scientific knowledge is still basic and there is much left to investigate
- During the past decades, quality of mathematical models within biology and agriculture have matured
- Therefore: Demands **and** means for extensive computer simulations!



Author: Luc Viatour

Context – Root water uptake

Plants transpire water, which needs to be taken up from groundwater

Understanding this process is relevant:

- Efficient watering of agricultural fields
- Avoid pesticide contamination

Relevant physical and biological processes:

- Water transport in soil
- Water transport within root network
- Interface between these systems

Author: Jörg Hempel

Context – Measurement and Simulation

Albeit scientific measurement is the measure of all things

- Experiments may be too expensive
- Method may be too intrusive
- Experiments may take months

Simulation serves as an appropiate means to aid scientific progress, and simulation software has been developed

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Water in Soil - Richards equation

Water transport in soil is governed by Richards equation

$$\partial_t \theta = \nabla (K(h) \nabla (h + z)) + S(h)$$

h : pressure head

θ : water content

S : sink term

K : hydraulic conductivity

z : vertical coordinate

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There is one-to-one-correspondence

$$\theta(h) = \theta_a + (\theta_m - \theta_a)(1 + |\alpha h|)^{-m}$$

constants :

$m, n, l, K_s,$

$\theta_a, \theta_m, \alpha$

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$m, n, l, K_s,$

$\theta_a, \theta_m, \alpha$

In fact, the highest-order term is far from being linear:

$$K(h) = K_S(1 - |\alpha h|)^{-ml}(1 - (1 - (1 + |\alpha h|)^{-\frac{mn}{n-1}})^{\frac{n-1}{n}})^2$$

Water in Soil - the Sink term

The sink term describes the water uptake.

It depends on humidity-dependent root properties (α) as well as the presence of roots (β).

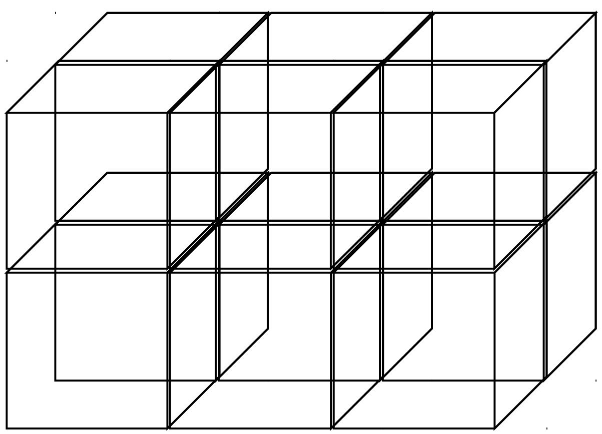
$$S(h) = \alpha(h)\beta(h)R$$

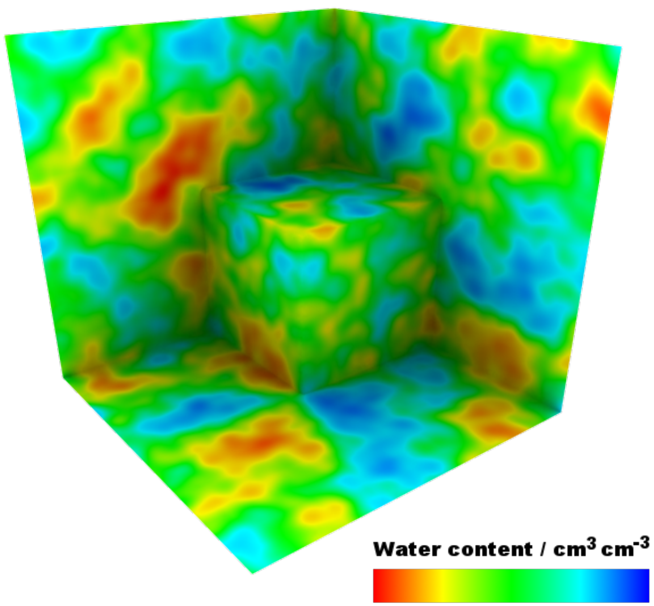
- $0 \leq \alpha \leq 1$ is a humidity-dependent factor which locally describes how much of the roots uptake capacity can be employed.
- $0 \leq \beta \leq 1$ is a uptake factor that locally describes how much a root segment contributes to the plants overall water uptake
- R is the transpiration rate at the collar of the root

Water in Soil - Finite Element Scheme

Replace continouos domain by rectangular mesh, and replace water content by discrete function

Main part consists of solving a linear system.

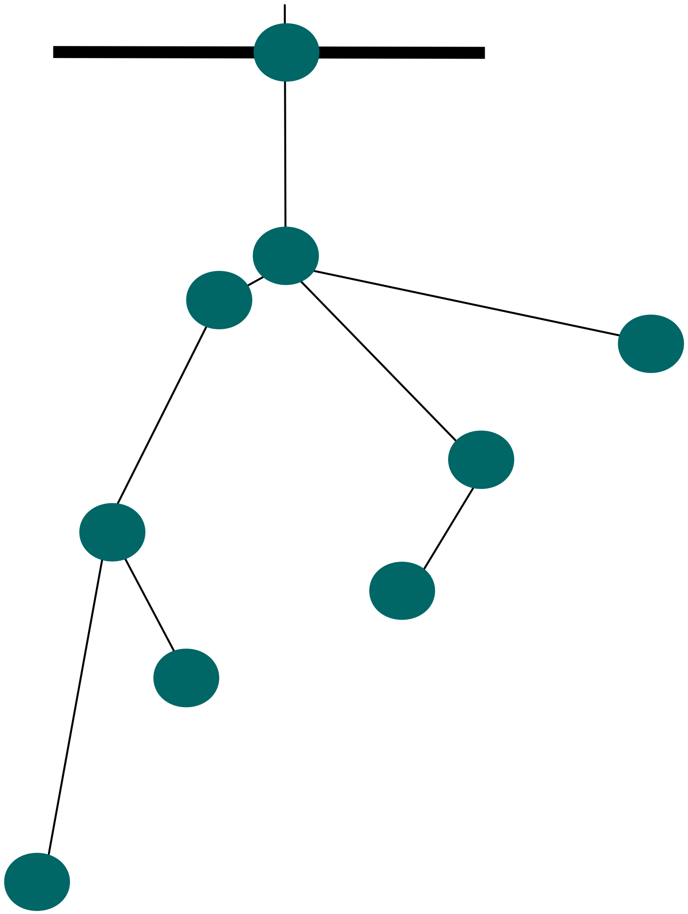




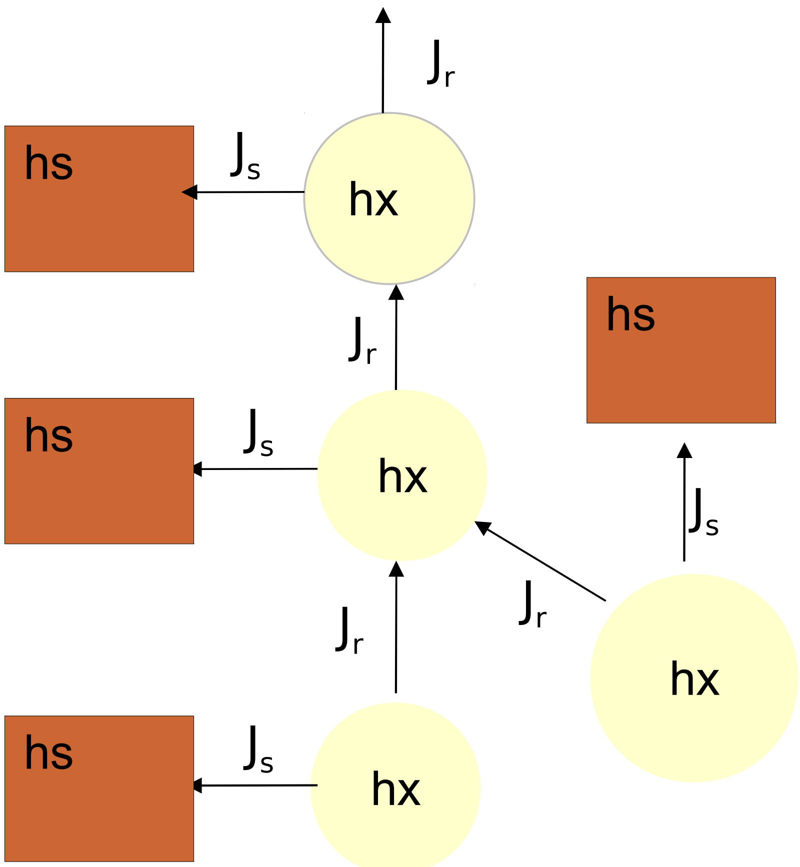
Author: Martin Galgon

Water in Roots - Doussan model

- Water transport within roots is described by the doussan model
- Root network is modeled as an tree-like structure of discrete nodes
- Each node carries information of its own water content, (and material properties)
- Water transport between root segments (and soil) is proportional to the negative gradient of water distribution



Water in Roots - Doussan model



J_r : root-root water flux

J_s : root-soil water flux

K_r : root-root conductivity

K_s : root-soil conductivity

h_r : root water pressure

h_s : soil water pressure

S : material constant

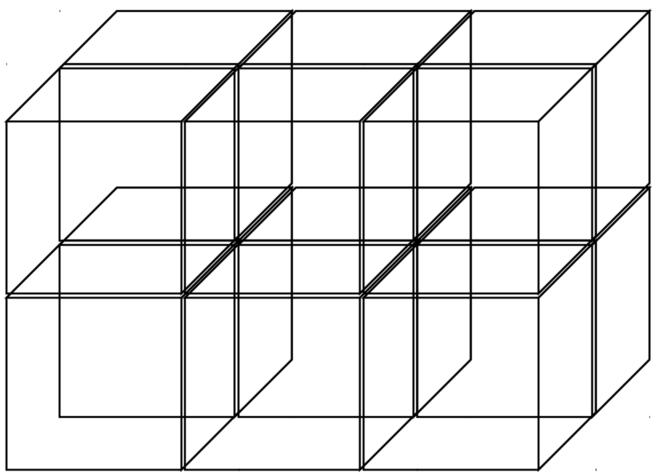
Induces a Linear System of Equations

$$J_x = -K_x(\partial_l h_x) \qquad J_r = -K_r S(h_s - h_x)$$

Coupled water flow model

SOIL

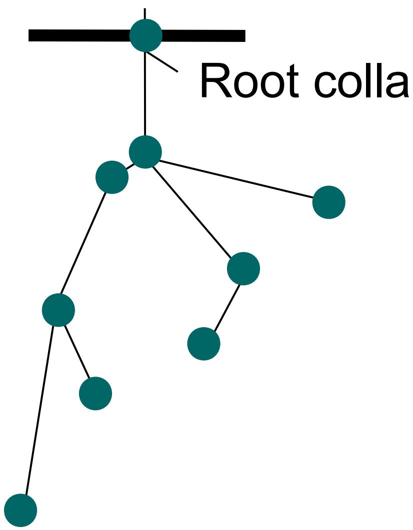
geometry: grid with hexaeders subdivided in tetraheders



numerics: Richards' equation with sink term S given by the soil-root fluxes

PLANT ROOT

geometry: tree-like structure with connected nodes



numerics: system of linear equations with boundary conditions given by the soil-root interface water potential and the plant collar flux

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Simulation Software developed

SWMS 3D
Water in soil
Serial simulation

- Somma e.a., 1992
- Fortran 77
- Water dynamics within soil
- Serial

Simulation Software developed

SWMS 3D
Water in soil
Serial simulation

ParSWMS
Water in soil
Parallel simulation

- Hardelauf, 2006, ICG IV
- C++89
- Parallel
- Employs
  - MPI
  - ParMetis (v.i.)
  - PetSc (v.i.)

A Closer look at parSWMS

- **ParMetis**
  - Finds an optimal distribution for the linear system amongst all processes
  - Flexible configurations possible
- **PetSc**
  - Flexibel and efficient library for parallel scientific computing
  - MPI-based
  - We employ a conjugated gradient method to solve the linear system of the water-in-soil-model

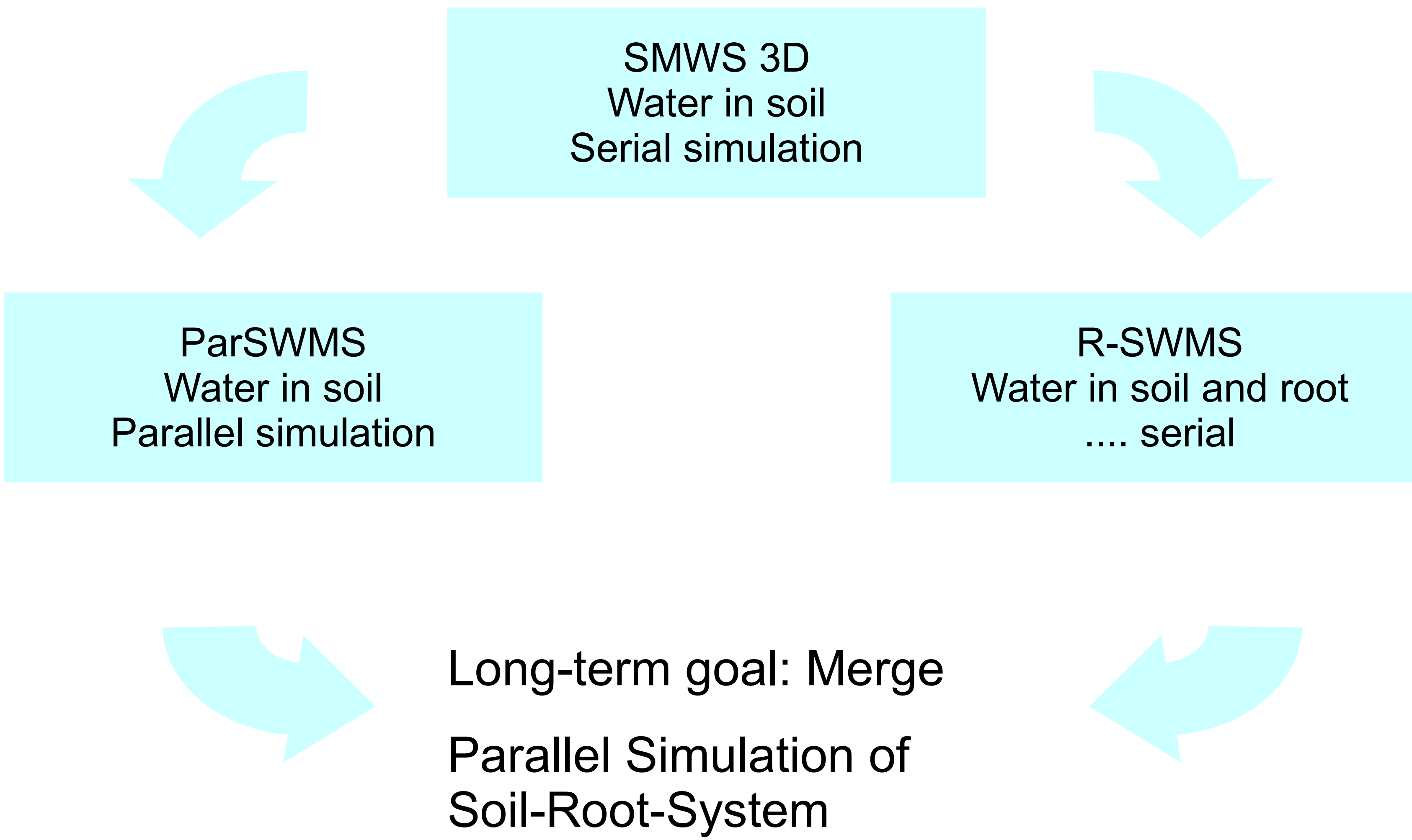
Simulation Software developed

SWMS 3D
Water in soil
Serial simulation

R-SWMS
Water in soil and root
.... serial

- Javaux, 2008
- Fortran90
- Serial like SWMS3D
- Large feature set to simulate soil-root dynamics

Simulation Software developed



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Objectives for my project

Enlarge the feature set of parSWMS.

Investigate prospects to several parallization strategies for the whole root-soil-system

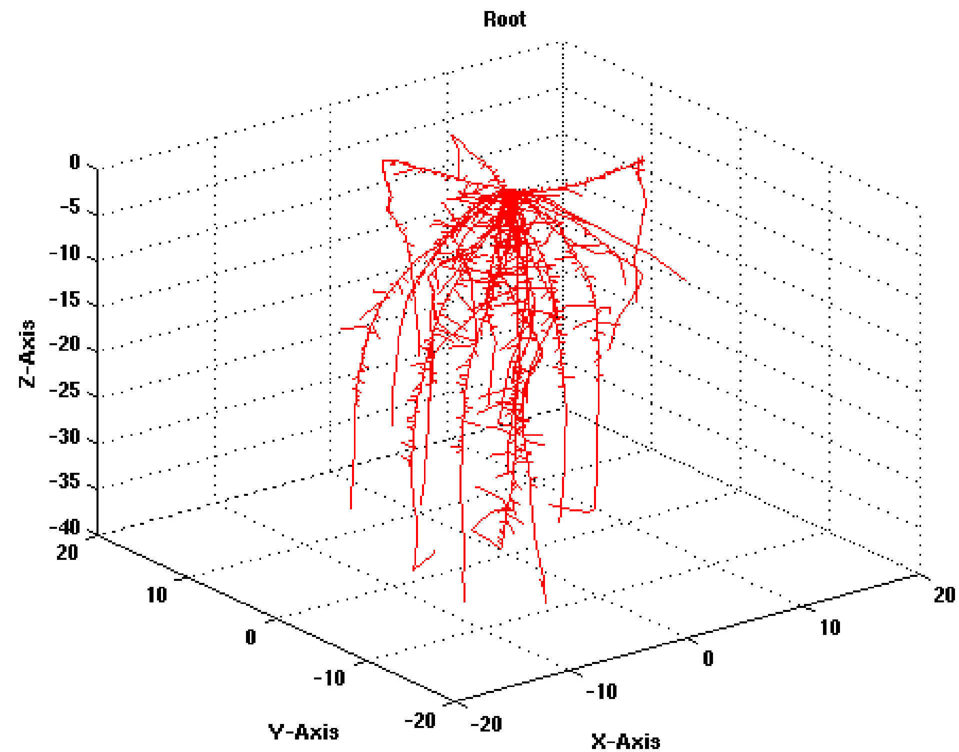
I. **Implement data structures to model roots in parSWMS (i.e. Migrate data structures from R-SWMS in an appropiate manner)**
II. **Implement root water uptake with respect to plant geometry**
    - **i.e. *„Roots affecting soil"***
III. **Benchmark the effect of several strategies**
    - ***Change the partition of the soil domain with regard to a given root geometry***

Note: The complete soil-root model has been far out of this projects scope

Just for your convenience...

All pictures to follow have been of one single example.

- Cubic bulk of soil
- 20cm x 20cm x 40cm
- 40 x 20 x 40 mesh resolution
- Homogenouos water saturation of 20%
- Root structure of age 45d



.... roughly an enviroment like within an experimental facility.

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  - II. Root water uptake
  - III. Benchmark distribution strategies
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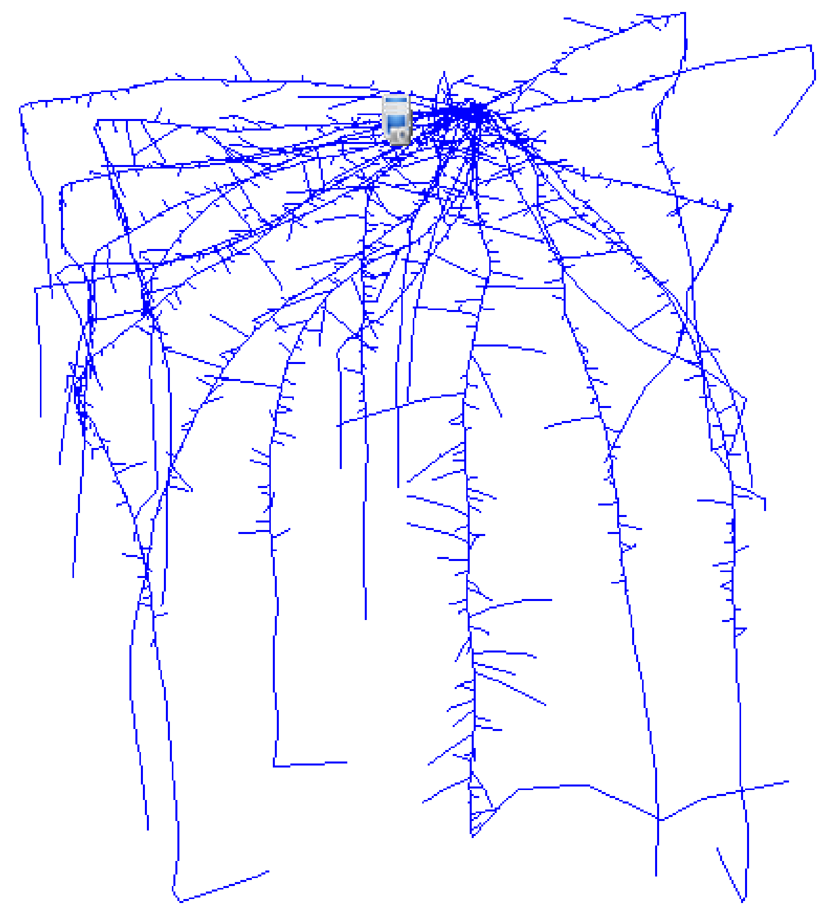
Root structure within parSWMS

- Root network modeled as (combinatorial) tree
- Implement as mix of adjacency list and double-linked list
- Currently each process has its own copy of the root structure
- Root parallelization strategy an open question as of now



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Root water uptake revisited

- Recall: The presence of roots in soil induces „dissappearance“ of water
- The uptake is modeled by the sink term „S“ in the Richards equation.
- At point of soil geometry, the sink term depends on material properties of soil, root segments and current water content
- Uptake ability is modeled by the term Beta

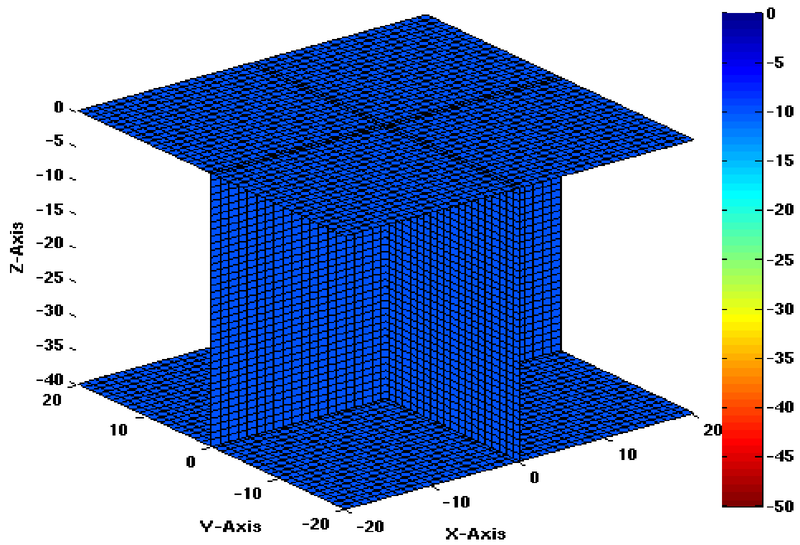
$$S(h) = \alpha(h)\beta(h)R$$

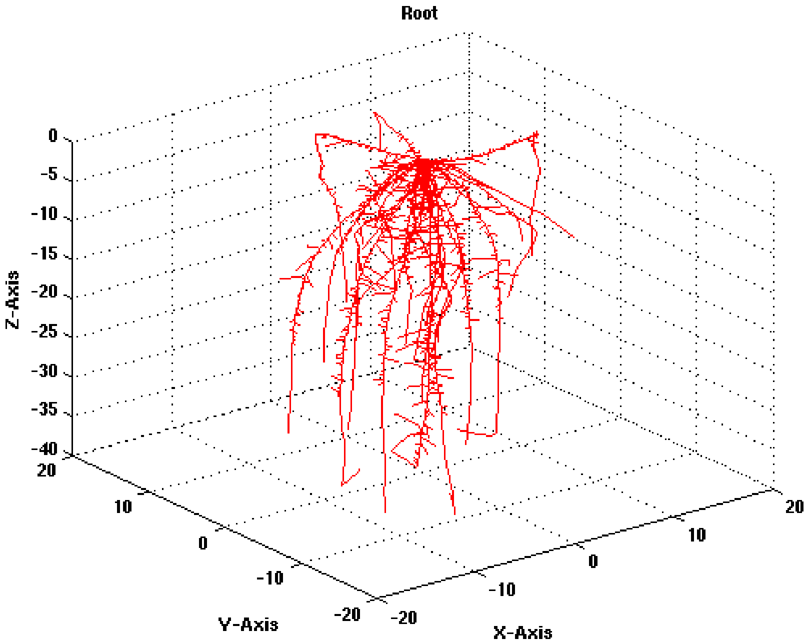
In parSWMS, you could set a sink distribution manually.

Now, parSWMS can build up this distribution with respect to a given root geometry.

Example: Water uptake visualized

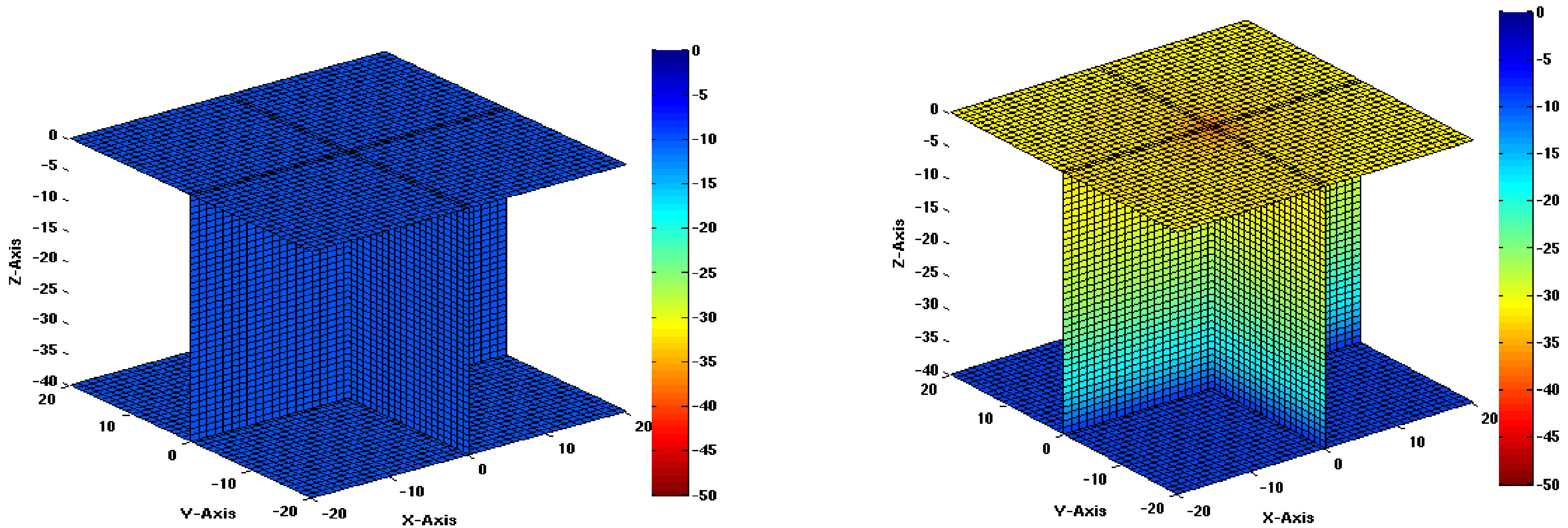
- Left Side: Depiction of initial homogenouos water distribution
- Right Side: Depiction of root structure again
- Simulation period of one month to be shown





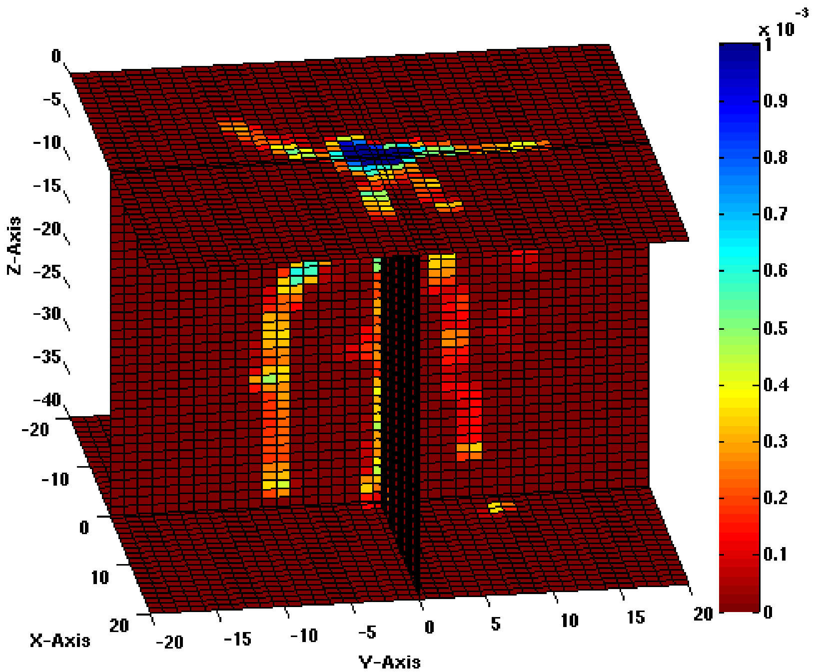
Example: Water uptake visualized

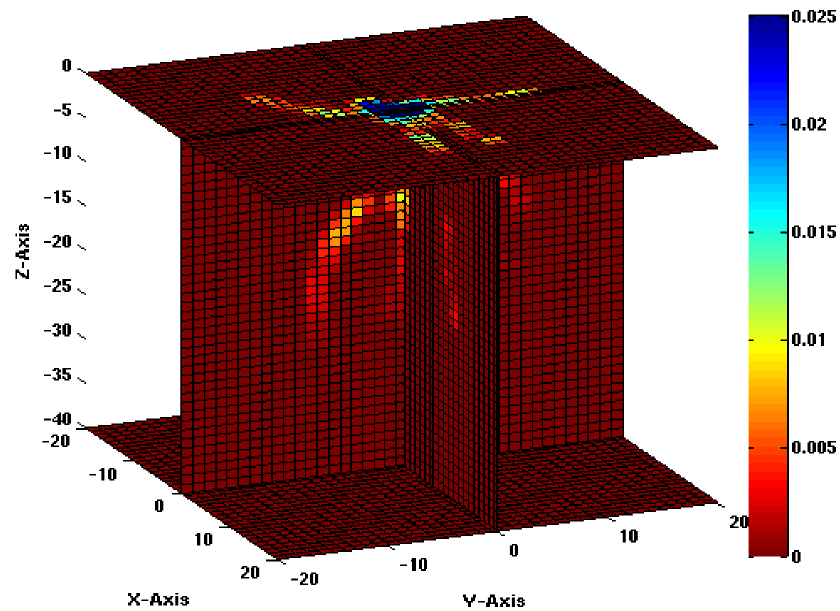
- In the upper parts of soil, centered around the root top, water saturation drops below a threshold such the plant cannot absorb anymore water.
- A residuum remains in the lower parts, the root cannot reach



Example: Water uptake visaulized

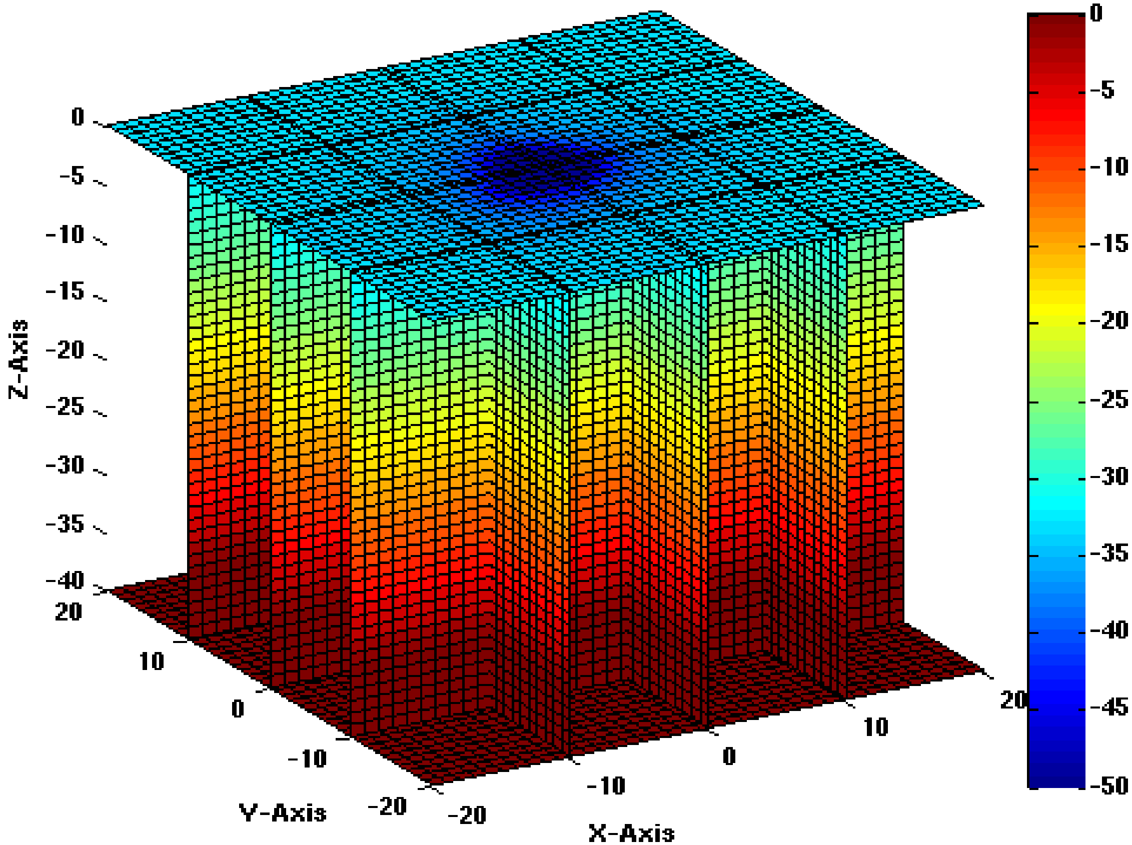
- Root water uptake right at start of simulation, when activity is highest
- Left side: Beta term
- Right side: Sink terms that result





A snapshot

- The state of the root system after 4 days.
- The qualitative evolution of the system can seen.



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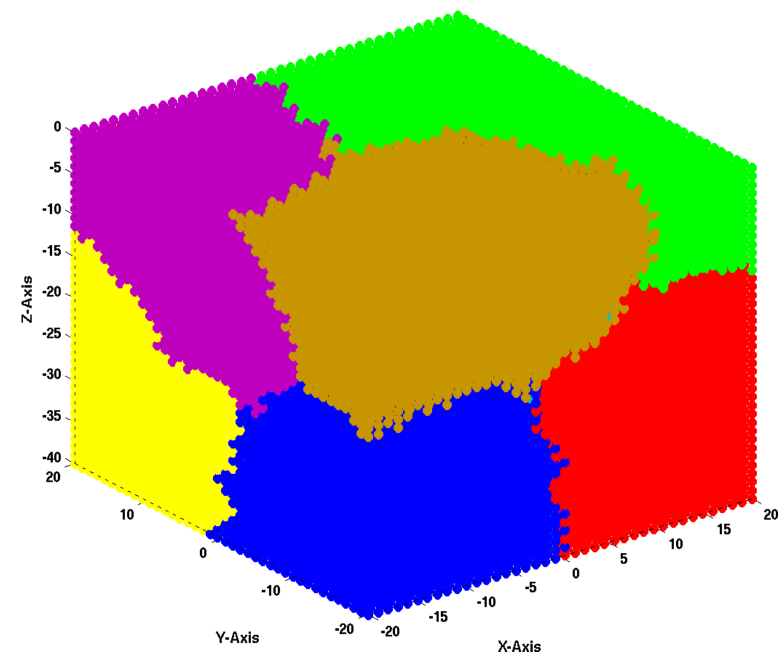
Grid partioning

- ParSWMS uses ParMetis library to find an optimal partition of the FE-mesh
- But when simulating whole soil-root-system, each subsystems optimal parallelization strategies may be counteracting each other.
- If influence of soil distribution by root geometry – how does the running time change?

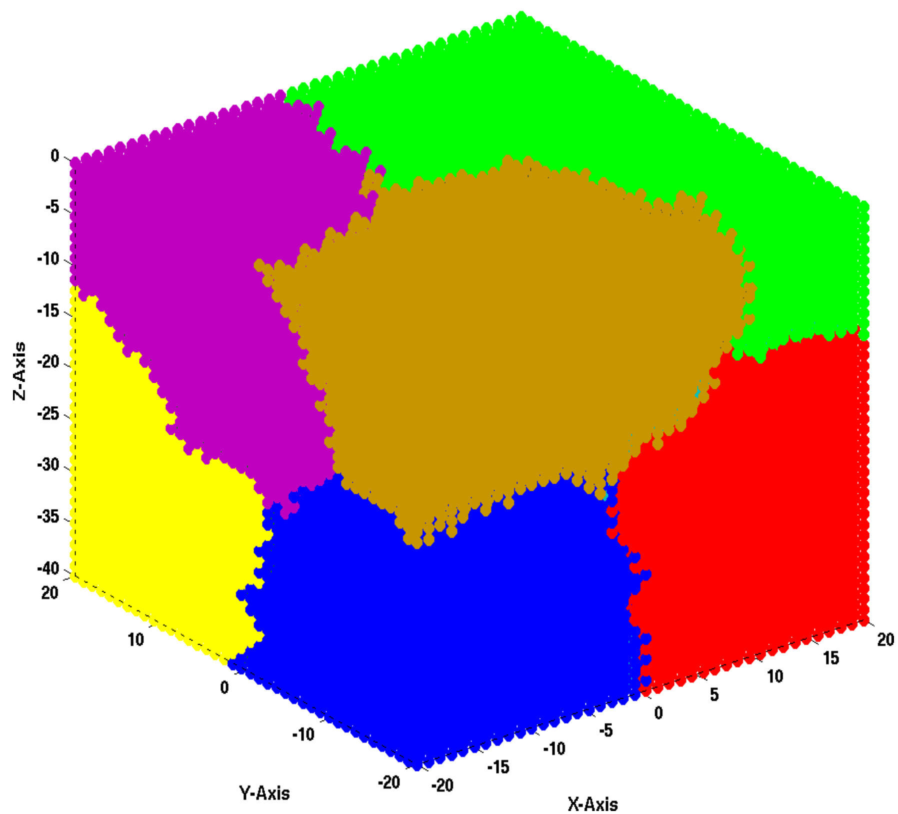


This can be done by assigning weights to the connections of neighbouring soil mesh nodes

Grid partioning

Strategies considered

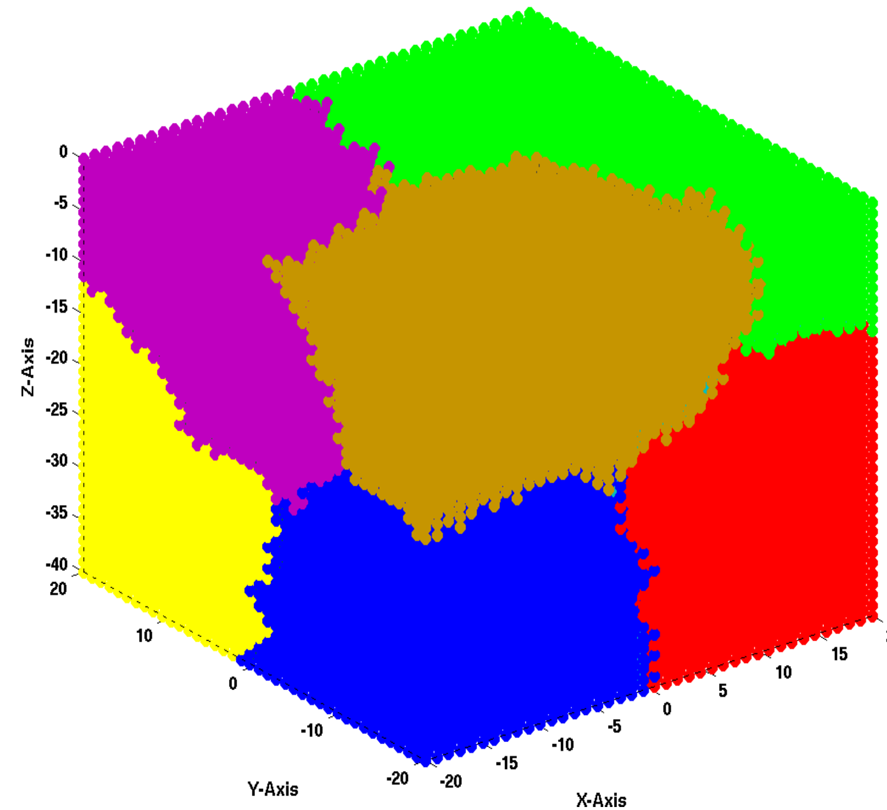
- **Keep normal partioning scheme**
- Avoid parting the soil where the root resides
- With multiple plants: part areas where roots of different plants reside



Grid partioning – Normal partition scheme

By default, the domain is partioned among the process in way that minimizes the communication during the solving.

In our example, with 8 processes, leads to about 9000+/-100 mesh nodes on each process



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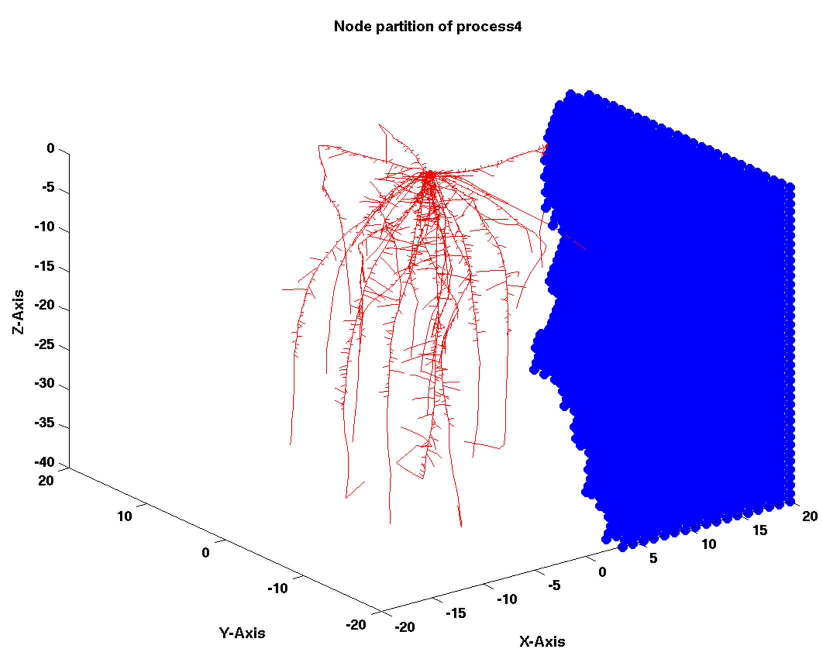
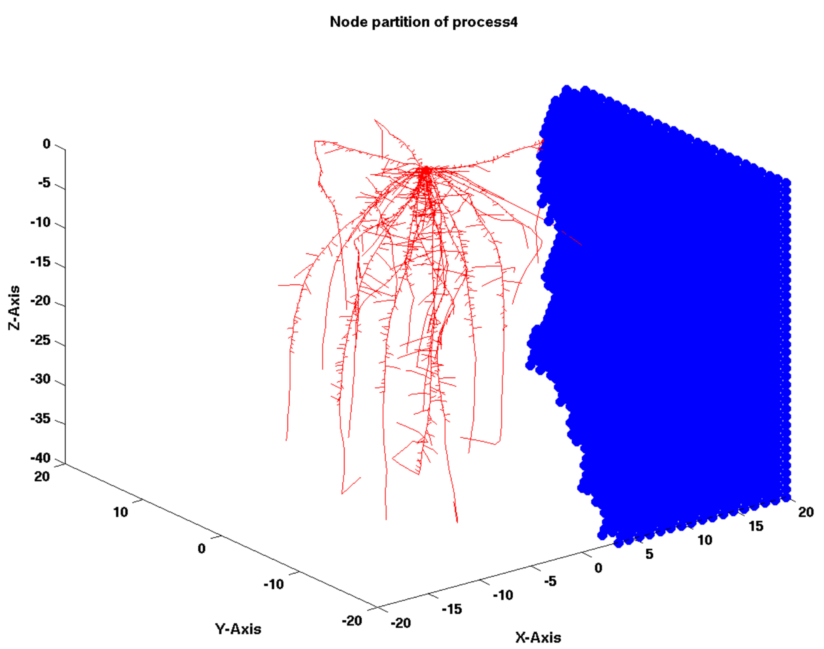


Grid partioning – Soil around Root on one process

- Might be useful, as root network often has significantly less degrees of freedom as soil network
- Easiest to implement
- Destroys scaling, as large part of geometry remains on one process



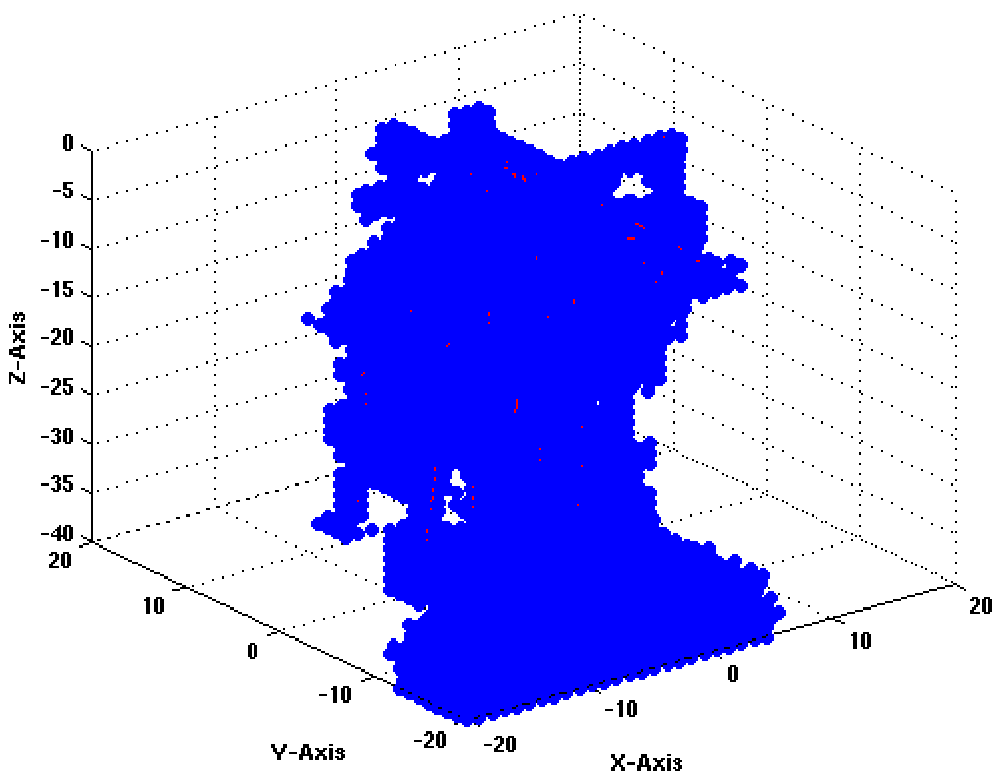
Our Example, with 8 processes again:

Ranges from 16000 to 5000 mesh nodes per process

How these partitions look like

Same scenario as before, with the effect amplified for the sake of illustration. 32 processes to be run.

Picture shows the process that manages the root-soil-interface

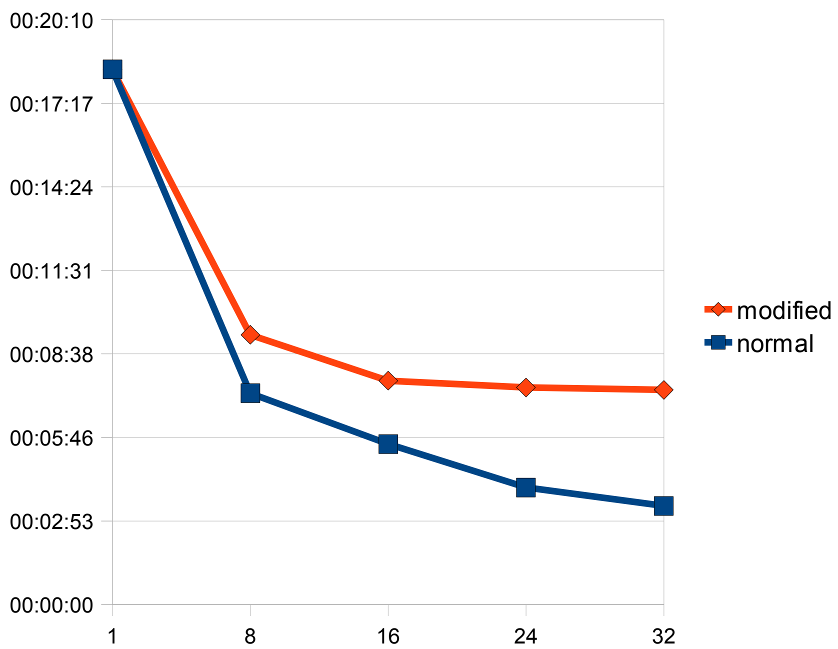


No matter how much processes are employed, there always remains a large „bulk“.

This in fact serializes the code!`

Comparison of running time

- Shown: Scenario simulated for 365d simulation time.
- Tested on Juropa.
- Running time [hh:mm:ss] plotted against number of processes [-].
- As expected the code is effectively serialized.



A slight change to the scenario

- It might be interesting to increase the grid-resolution.
  - **More** performant, as soil can be finer parted?
  - **Less** performant, as interaction face enlarges?
- Altered our scenario to a resolution of 400 x 200 x 400

A slight change to the scenario

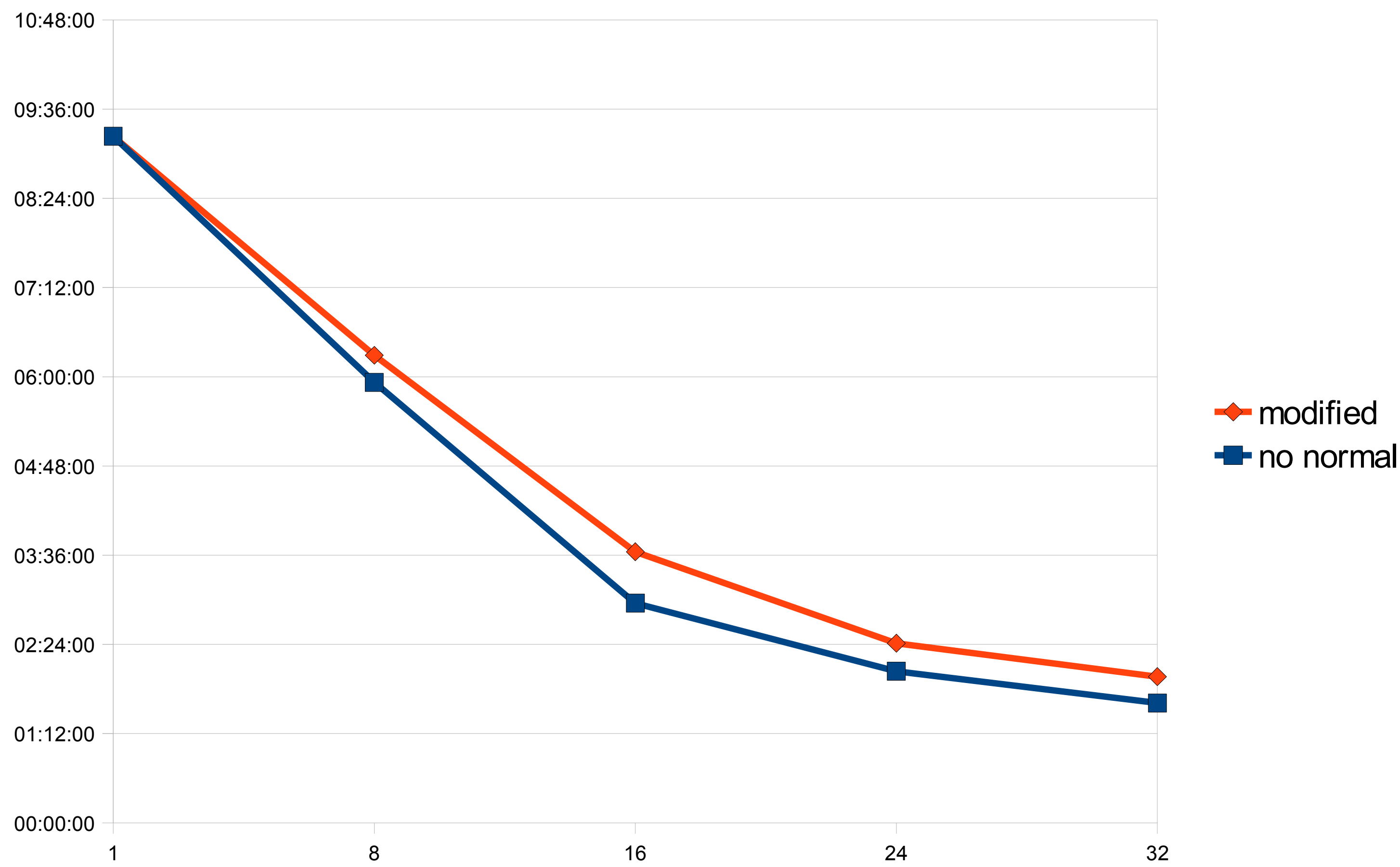
- It might be interesting to increase the grid-resolution.
  - **More** performant, as soil can be finer parted?
  - **Less** performant, as interaction face increases?
- Altered our scenario to a resolution of 200 x 200 x 200

Again

- Tested on Juropa.
- Running time [hh:mm:ss] plotted against number of processes [-].
- Plot to follow....

Comparison of running time

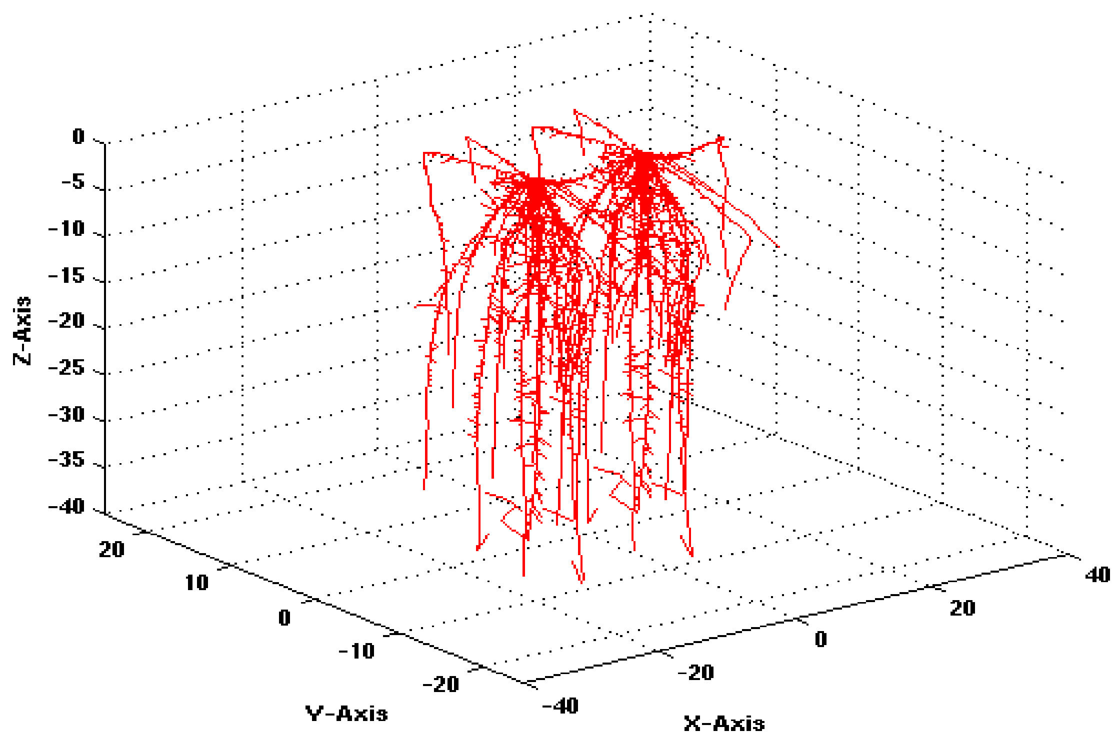
- Result looks positive!



Grid partioning

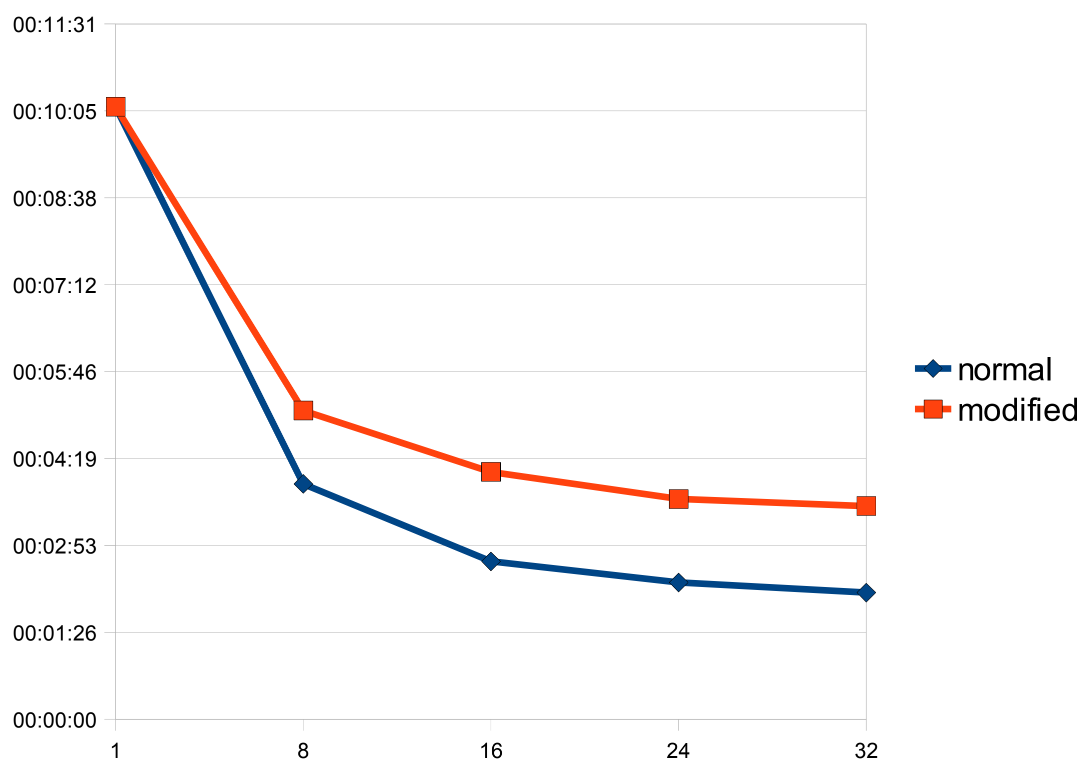
Strategies considered

- Keep normal partioning scheme
- Avoid parting the soil where the root resides
- **With multiple plants: part areas where roots of different plants reside**



Comparison of running time

- Shown: Scenario simulated for 150d simulation time
- Tested on Juropa
- Running time [hh:mm:ss] plotted against number of processes [-]
- Effective serialization again, yet not that strong



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Goals achieved

- *(cleaned up code…)*
- Introduced root data structures in parSWMS
- Implemented parallel root water uptake
- Implemented distribution strategies
- Benchmarked the effect of these features
    - If the root-penetrated soil resides on only one process, the scaling is effectively lost
    - Increasing the grid resolution dampens this loss of performance
    - In the multiple-plant scenario, this effect is less drastically.

Outlook and Prospects

Widen the scope of features simulated

- Implement root growth simulation
- Implement root water transport (Doussan model)
- Parallize the root simulation, too

Improve given functionality

- MPI and OpenMP?
- Change the solver
- Implement grid adaptivity

Finally ....

Thanks for your attention!

Questions welcome!

Backup slides

The following slides are intended as backup only.

They are solely suited to provide basic information on additional questions.

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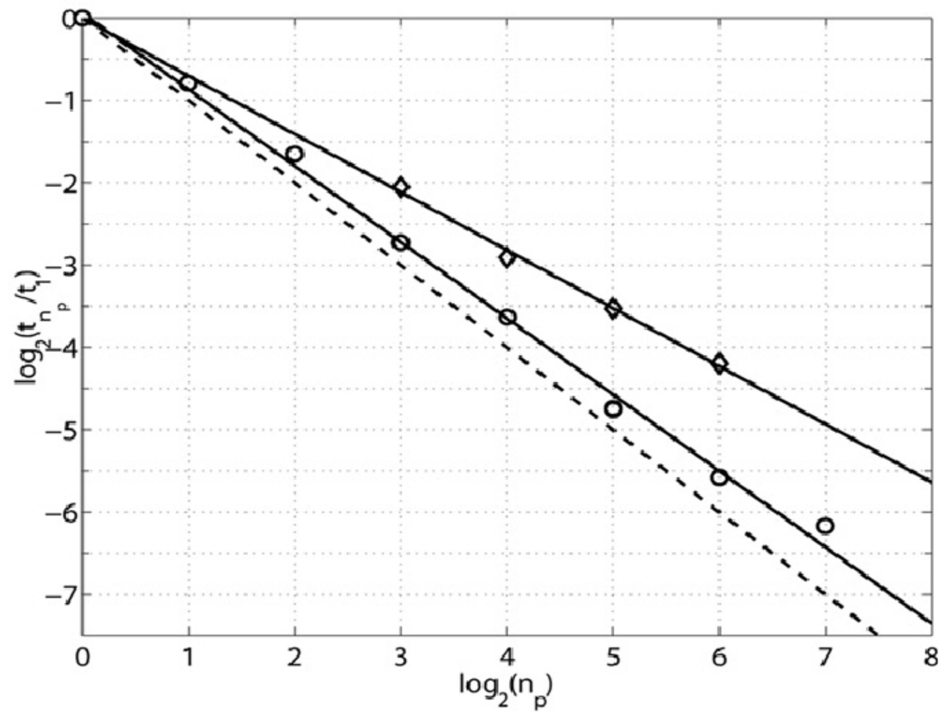
Backup : Scaling of parSWMS

- Numerical experiments have been conducted
- Test has taken place on jump
- Near optimum scaling up to 32 processes.



Backup : Root water uptake

These two systems have to be coupled, which introduces non-trivial numerical methods

- Water „disappears“ from soil into roots
- Ability of the plant to uptake water is influenced by the soils humidity itself non-trivially
- Conditions outside soil to be taken into account...
- At each time step, soil and root system are solved by turns, until solution is found

Backup: Logscale

- For the scenario mentioned, a loglog-plot of number of processors against running time. First Benchmark.