

Coupled water and energy transfers in porous media with freeze/thaw: permaFoam, a massively parallel OpenFOAM[®] solver.

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Transfers on boreal continental surfaces: role of the permafrost ?



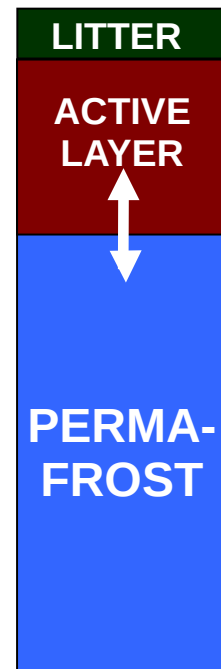
Problematic: climate change and weathering in boreal areas with a continuous permafrost

Studied area:

- Central Siberia, sub-watersheds of the Nizhnyaya Tunguska
- homogeneous vegetation cover and lithology
- main spatial variability: south aspected / north aspected slopes

Goals:

- Influence of seasonal freeze/thaw of the active layer on the geochemical fluxes related to weathering
- Impact of the interannual variations of these cycles due to climate change



Methodological approach :

Mechanistic modeling of thermal and hydrological transfers from the pedon scale to the **experimental watershed scale**

- Time scales : days to tens of years
Space scales : 1 m² to 10's of km²

First case of application: permafrost annual dynamics in Kulingdakan watershed

Mechanistic modeling of thermal and hydrological transfers

Numerical modelling of coupled transfers of water and energy with phase change within soils: **complex problem, broad associated literature**

(e.g.: Kennedy and Lielmezs, 1973, Harlan 1973, Guymon and Luthin 1974, Jame and Norum 1980, Seregina 1989, Boike *et al.*, 2003, Hansson *et al.*, 2004, McKenzie *et al.*, 2007, Weismüller *et al.*, 2011, Painter 2011, Frampton *et al.*, 2011, Grenier *et al.*, 2012, Rivière 2012, Endrizzi *et al.*, 2013, Kurylyk *et al.*, 2014, Karra *et al.*, 2014, Frederick and Buffet, 2014 ...)

Large computation times may be encountered: need of HPC methods.
Use of **massively parallel computation** is necessary
(e.g.: Painter *et al.*, 2013, Walvoord et Kurylyk, 2016).

=> a devoted solver with the **open source, generalist CFD tool**

OpenFOAM®: permaFoam

OpenFoam[®]: an open source CFD tool box for HPC

Developed in C++

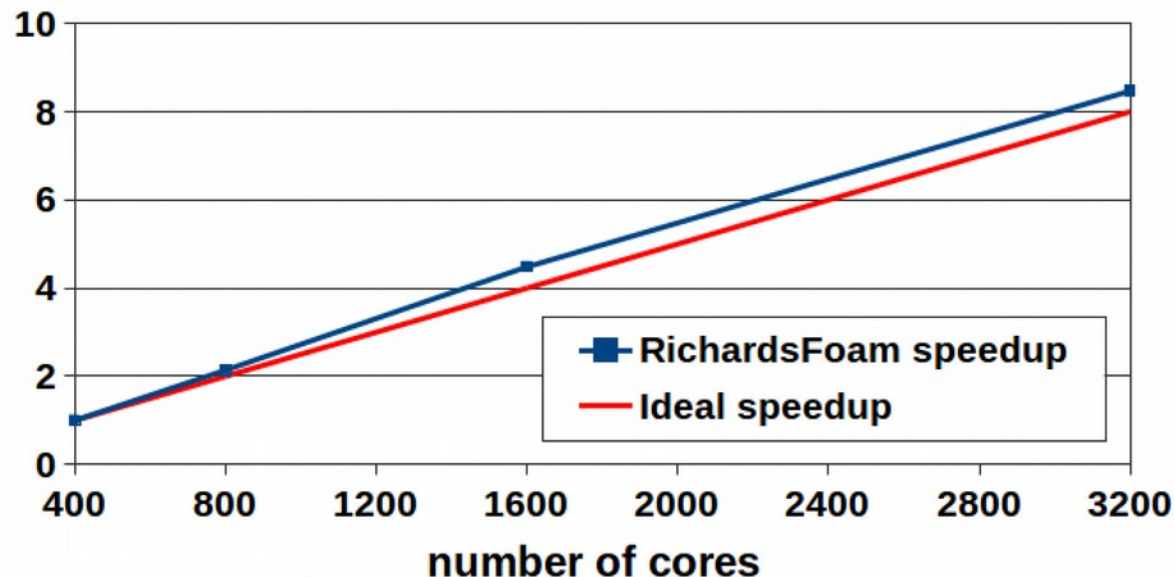
Finite volumes

Allow **multiphysics modelling**

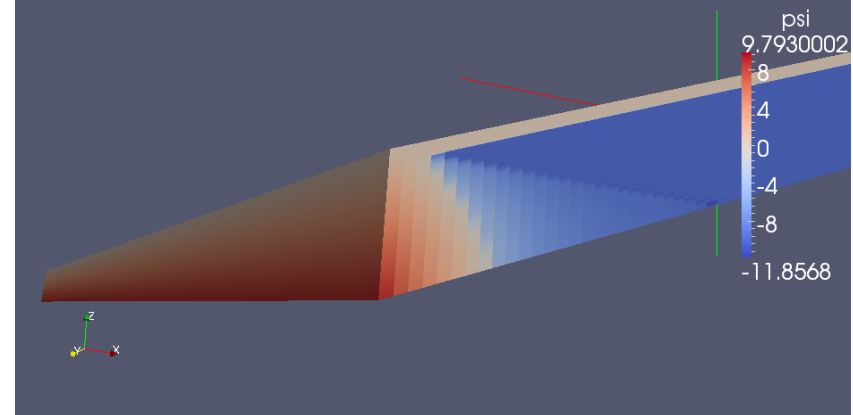
Enable to implement home-made solvers

Designed for **High Performance Computing**
(especially massively parallel computing)

OF for hydrological transfers in soil: RichardsFoam
(Orgogozo *et al.*, CPC 2014, Orgogozo, CPC 2015)



A RichardsFoam Test case :infiltration of rain in a parallelepipedic 3D slope



RichardsFoam parallel performances:

- **1.2 billion cells mesh**
- **From 400 to 3200 cores**
- **Scaling curve obtained on EOS**
(www.calmip.univ-toulouse.fr)

permaFoam: considered conservation equations

3D coupled heat and water transfers in variably saturated porous media, taking into account evapotranspiration and freeze/thaw of the poral water (Orgogozo *et al.*, under review):

couplings, non linearities

Richards equation with evapotranspiration:

$$C_H(h) \frac{\partial h}{\partial t} = \nabla \cdot (K_H(h, T) \nabla (h + z)) + Q_{AET}(h, T)$$

Thermal transfer equation with freeze/thaw:

$$\frac{\partial (C_{T_{eq}}(h, T) T)}{\partial t} + \nabla \cdot (\mathbf{v}(h, T) C_{T_{liquid}} T) = \nabla \cdot (K_{T_{eq}}(h, T) \nabla T) + L \frac{\partial \theta_{ice}(h, T)}{\partial t}$$

**Stiff problems, non linearities, couplings, few references solutions:
InterFrost Benchmark (C. Grenier, wiki.lsce.ipsl.fr/interfrost)**

permaFoam: numerical strategy

Couplings: - sequential operator splitting approach

- impedance factor approach for permeability in frozen state

Non linearities: - a Picard loop for each equation

- temporal shift of the latent heat term

- adaptive time steps based on Picard loops convergence

Richards equation with evapotranspiration:

$$C_H(h) \frac{\partial h}{\partial t} = \nabla \cdot (K_H(h, T) \nabla (h + z)) + Q_{AET}(h, T)$$

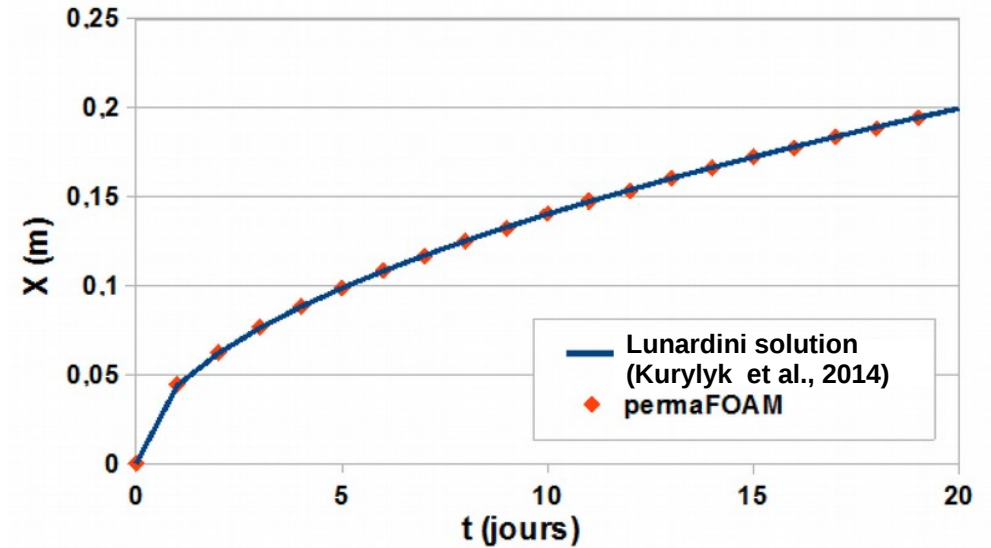
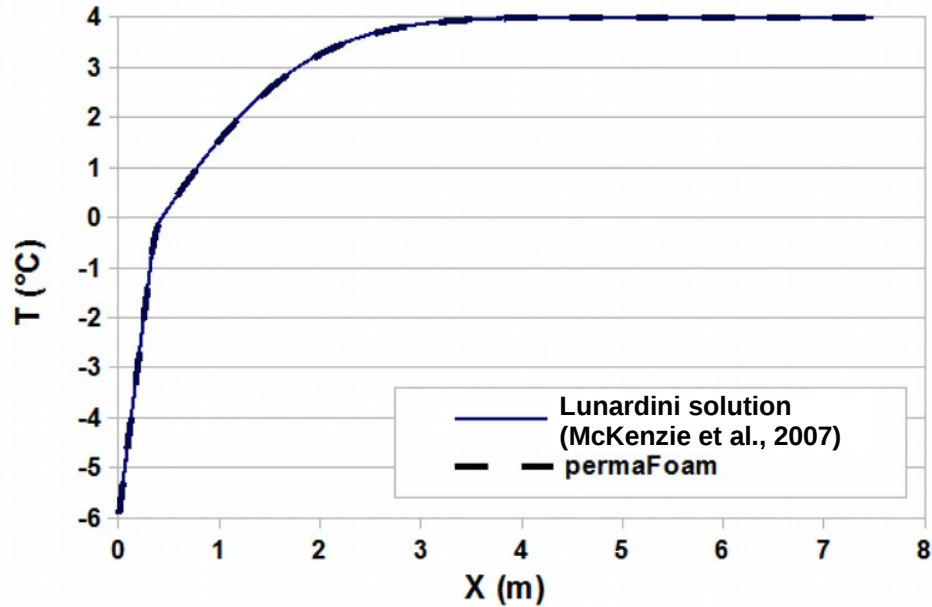
Thermal transfer equation with freeze/thaw:

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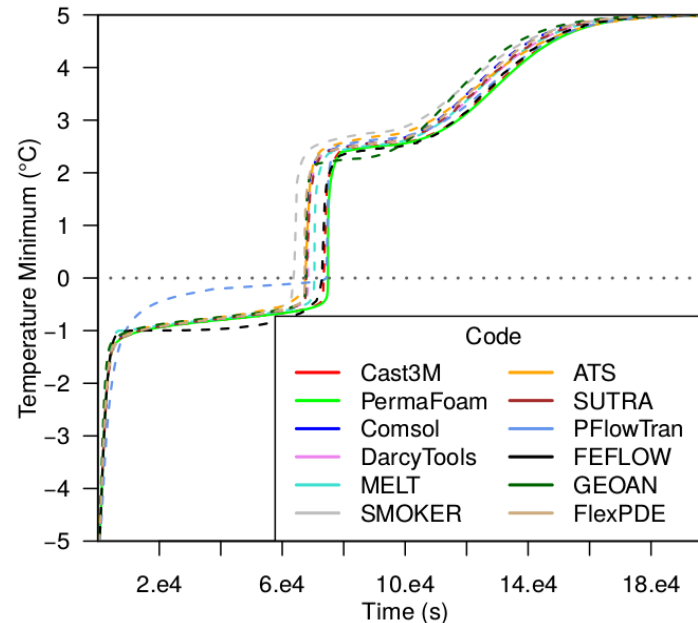
Stiff problems, non linearities, couplings, few references solutions:

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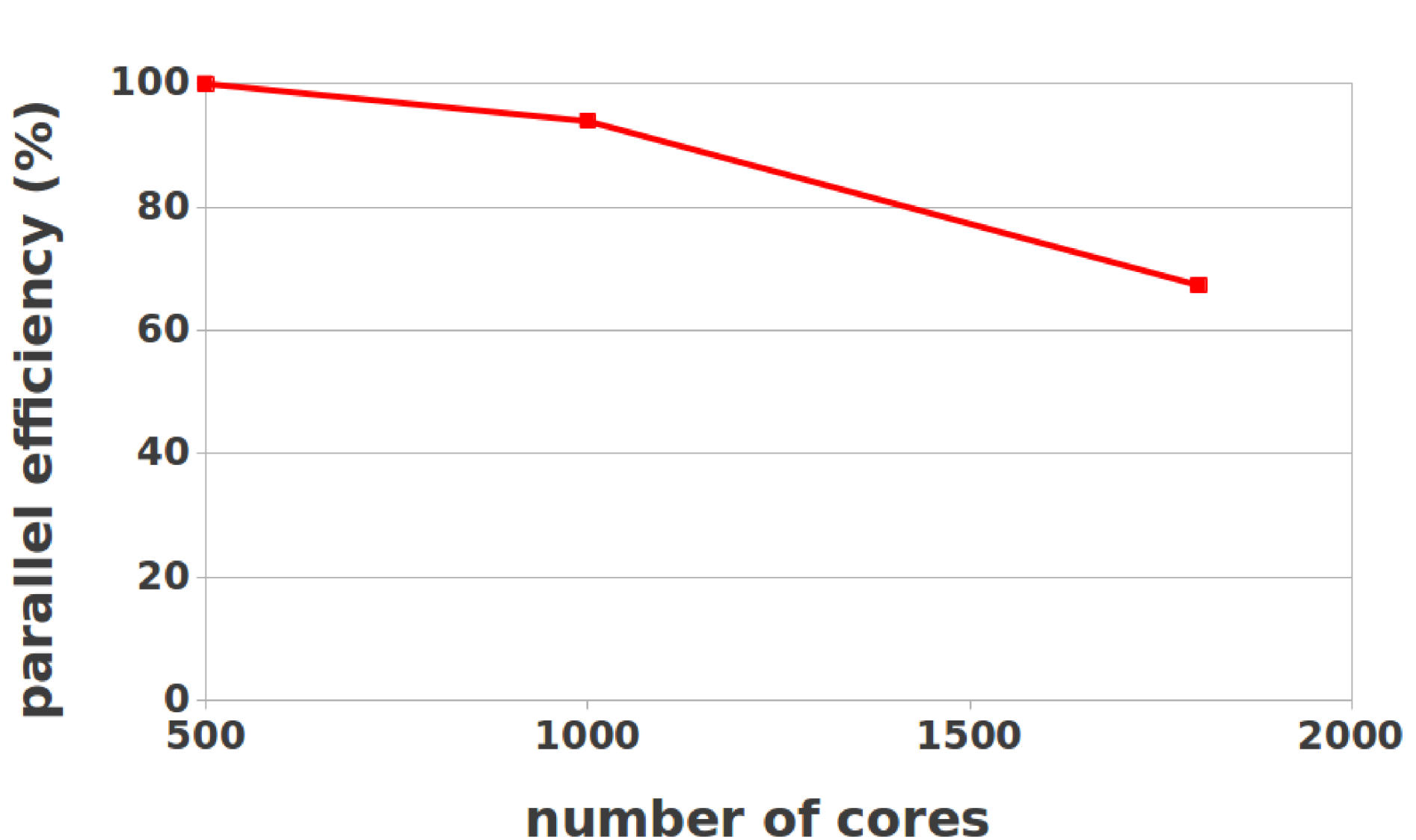
Validation and benchmarking



Interfrost benchmark: wiki.lsce.ipsl.fr/interfrost
 (Grenier et al., AGU 2013, EGU 2015, ICOP 2016, EGU 2017)



Parallel behaviour

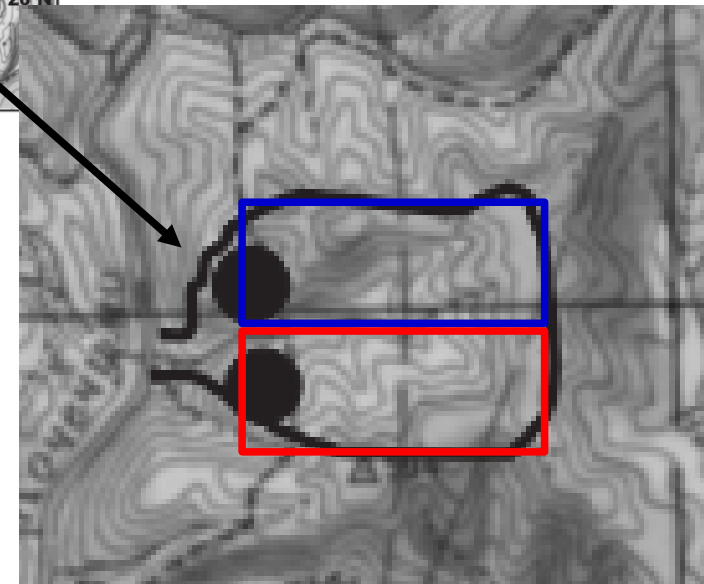
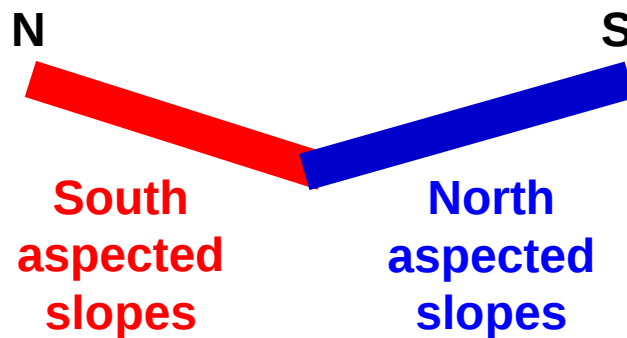


Reasonable parallel performances, likely limited by the small size of the considered test cases (meshes of only 10 millions cells)

Kulingdakan: a stream in a continuous permafrost area

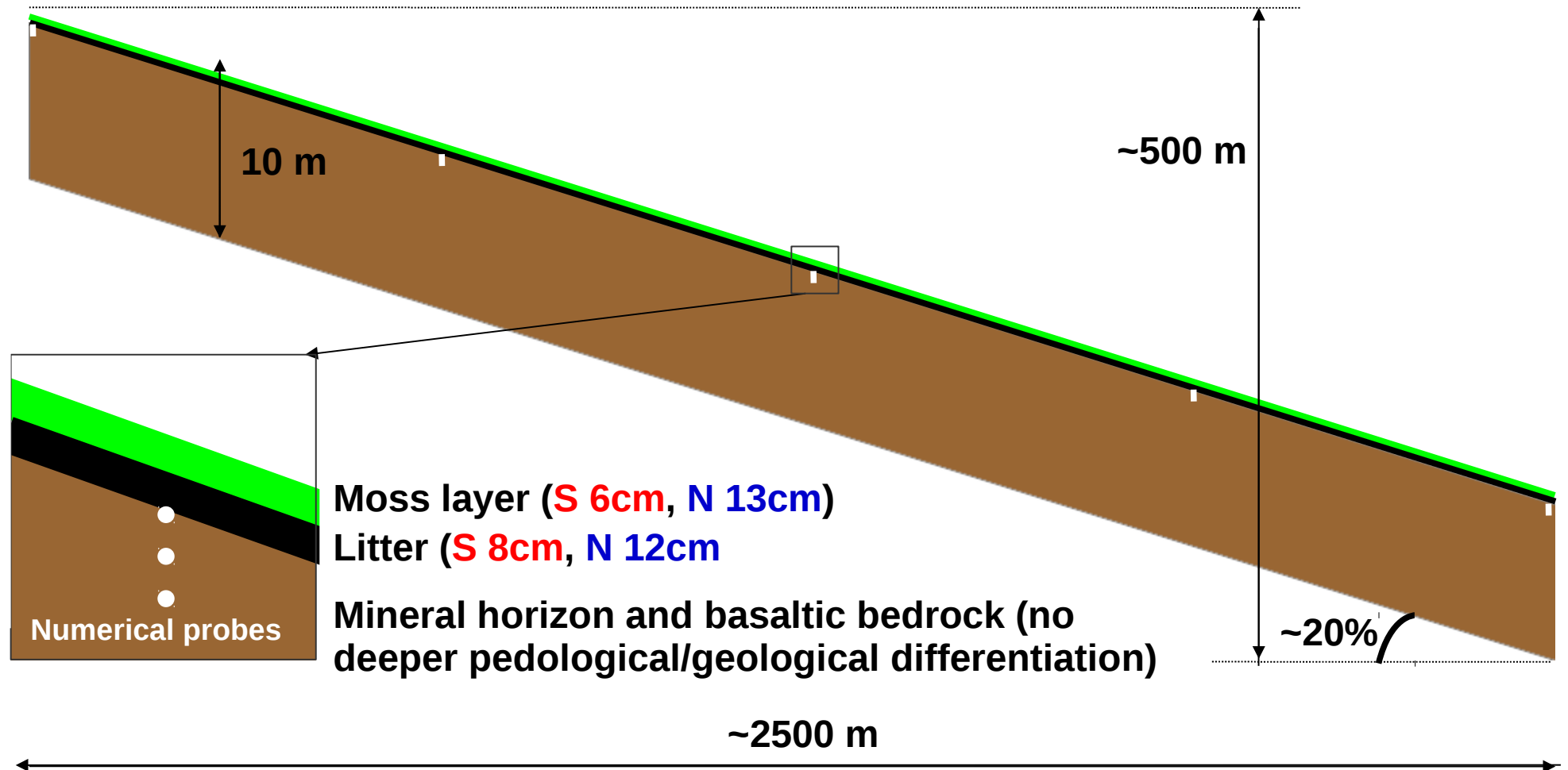


(according to Prokushkin et al., 2005)



Orientation and shape of the **Kulingdakan watershed** (e.g.: Prokushkin et al., 2005, Viers et al., 2015) well suited for a **dual (N/S) 2D simplified representation**

2D representation of the slopes of the catchment



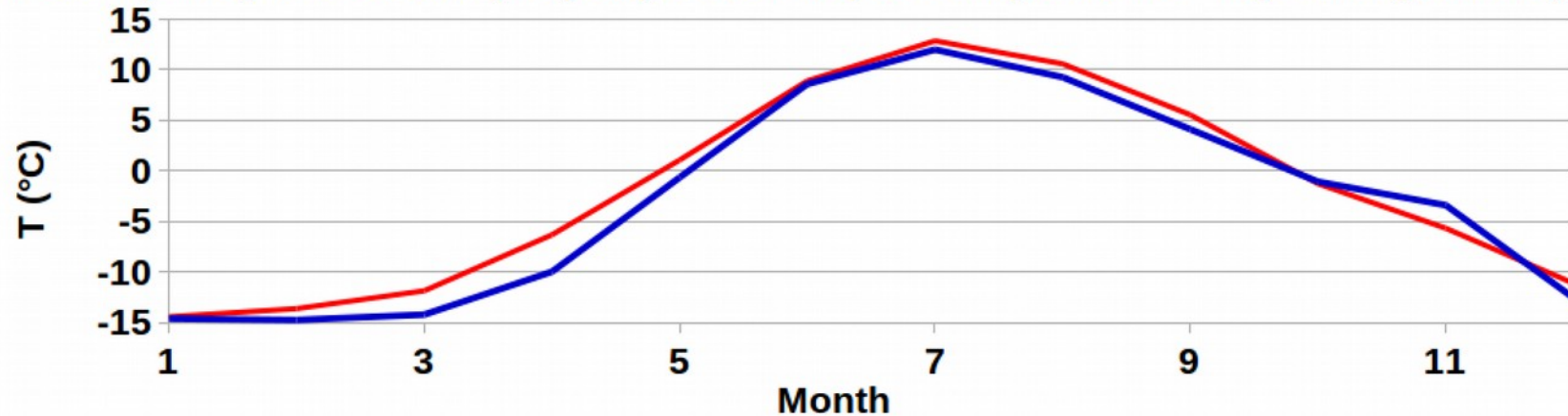
Mesh:

2.5 millions of cells, thicknesses from $5 \cdot 10^{-3}$ m (top) to 0.2 m (bottom), 0.2 m width

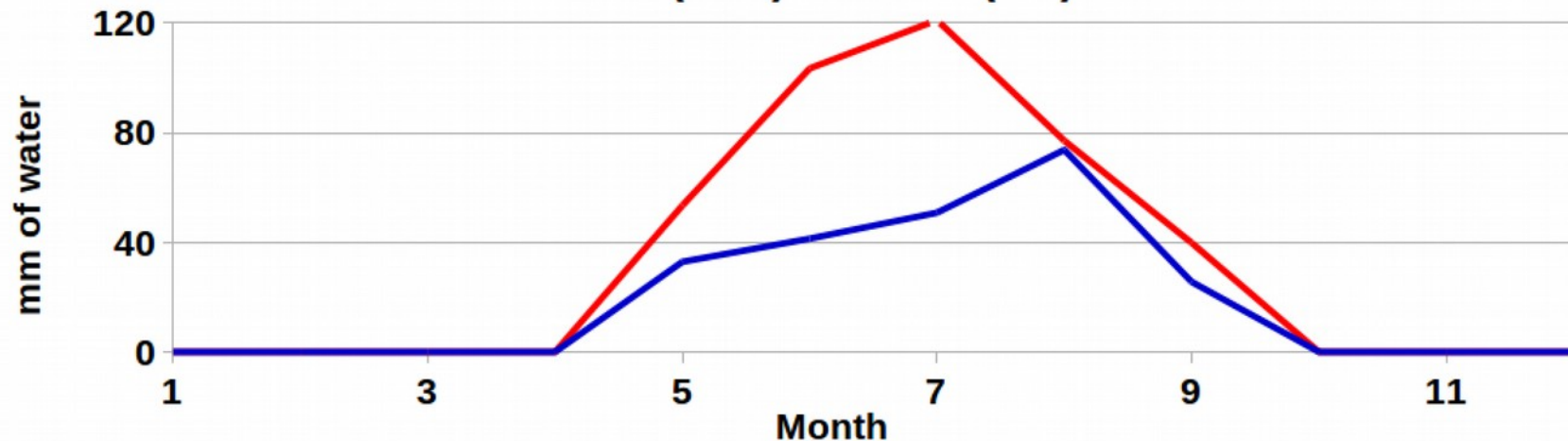
Climatic conditions

Multi-annual averages of the **observed monthly forcings**

North (blue) and south (red) aspected slopes temperature - top of organic layer



Rain (blue) and PET (red)



Input data for a transient modeling in the N/S aspected slopes along an hydrological cycle.

Temperatures in the mineral horizon

Reasonable agreement between observations and modelling results

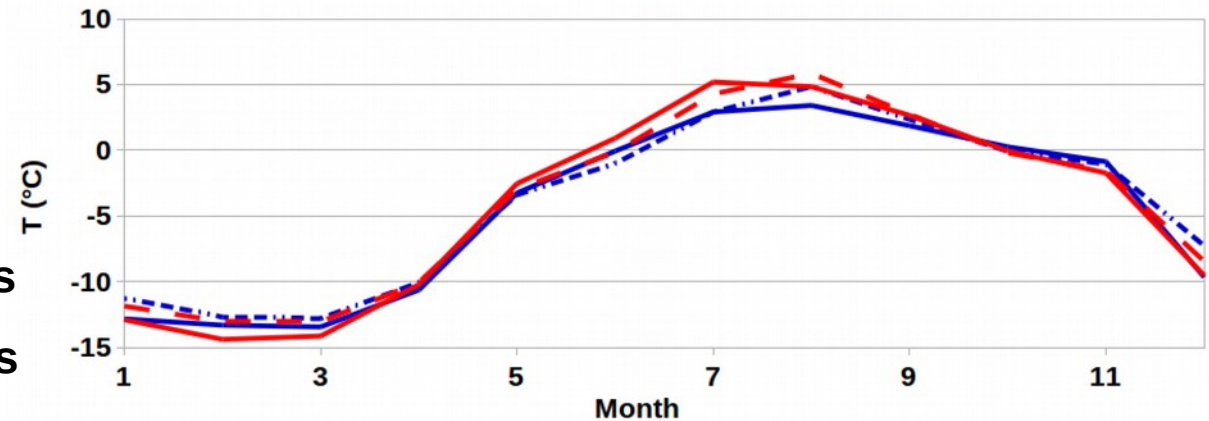
Generally, observations warm up and cool down faster than modeling results

→ macroporosities, thermal properties estimations, ... ?

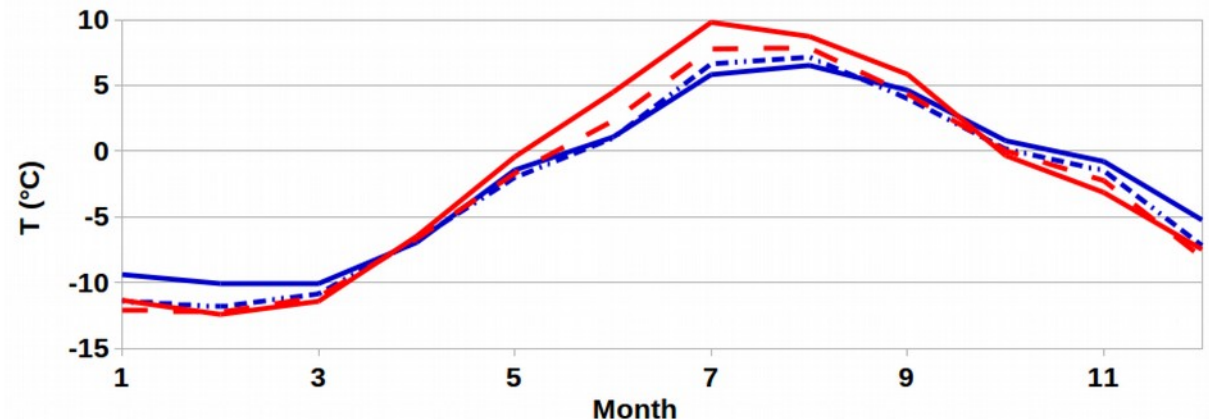
Computational facts:

- ~ 10 000 CPU hours
- Mesh: ~ 2 400 000 cells
- Max time step: 5s to 1h
- Computational resources: From 20 cores to 100 cores requests (processors: Intel(r) IVYBRIDGE 2,8 Ghz 10-cores) on **CALMIP** cluster EOS (www.calmip.univ-toulouse.fr)

Soil temperature at different depths: north aspected slopes



Soil temperature at different depths: south aspected slopes



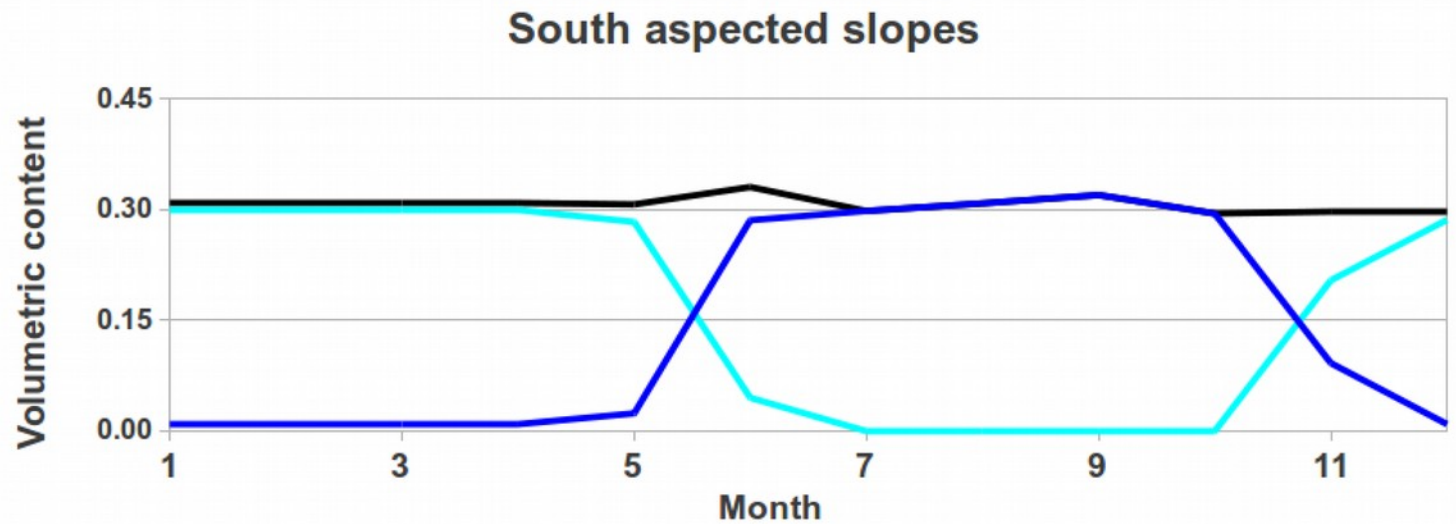
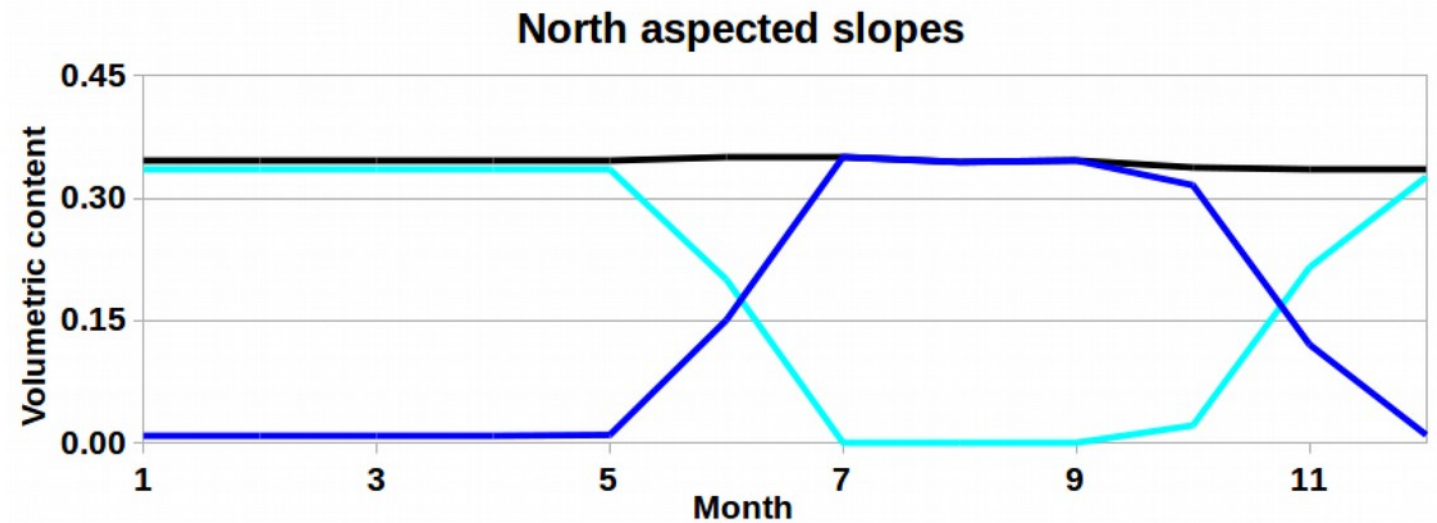
— Mineral horizon – 10cm (measured) - - - Mineral horizon – 10cm (computed)
— Mineral horizon – 20cm (measured) - - - Mineral horizon – 20cm (computed)

Water content in mineral horizon

Numerical results

20cm depth within
the mineral horizon

As expected, south
aspected slopes
are dryer and thaw
faster than north
aspected slopes



— liquid

— ice

— total

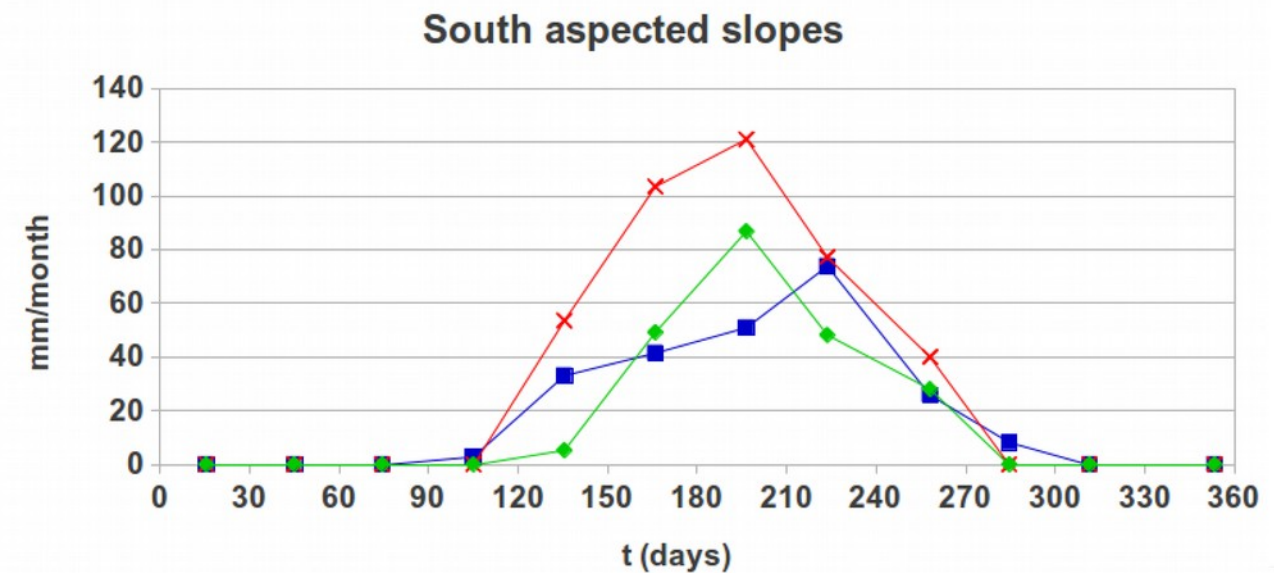
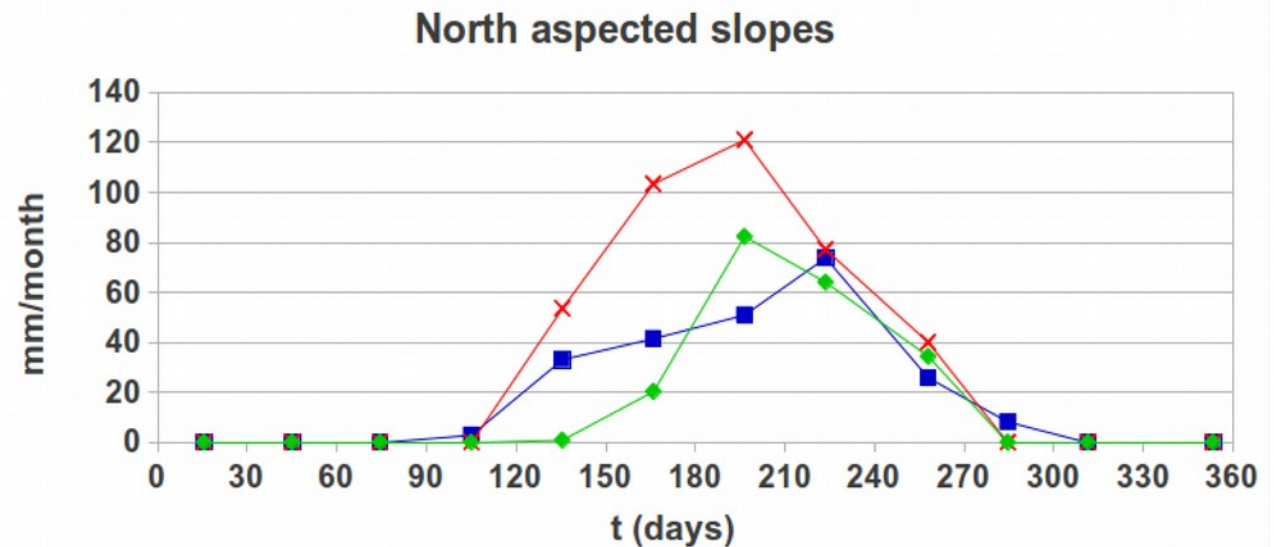
Actual evapotranspiration

Rain, PET: forcings

AET: numerical results

Two limitations to AET:
frost and dryness

South aspected slopes experienced 1 more month of «drying conditions» (AET > rain) as compared with north aspected slopes

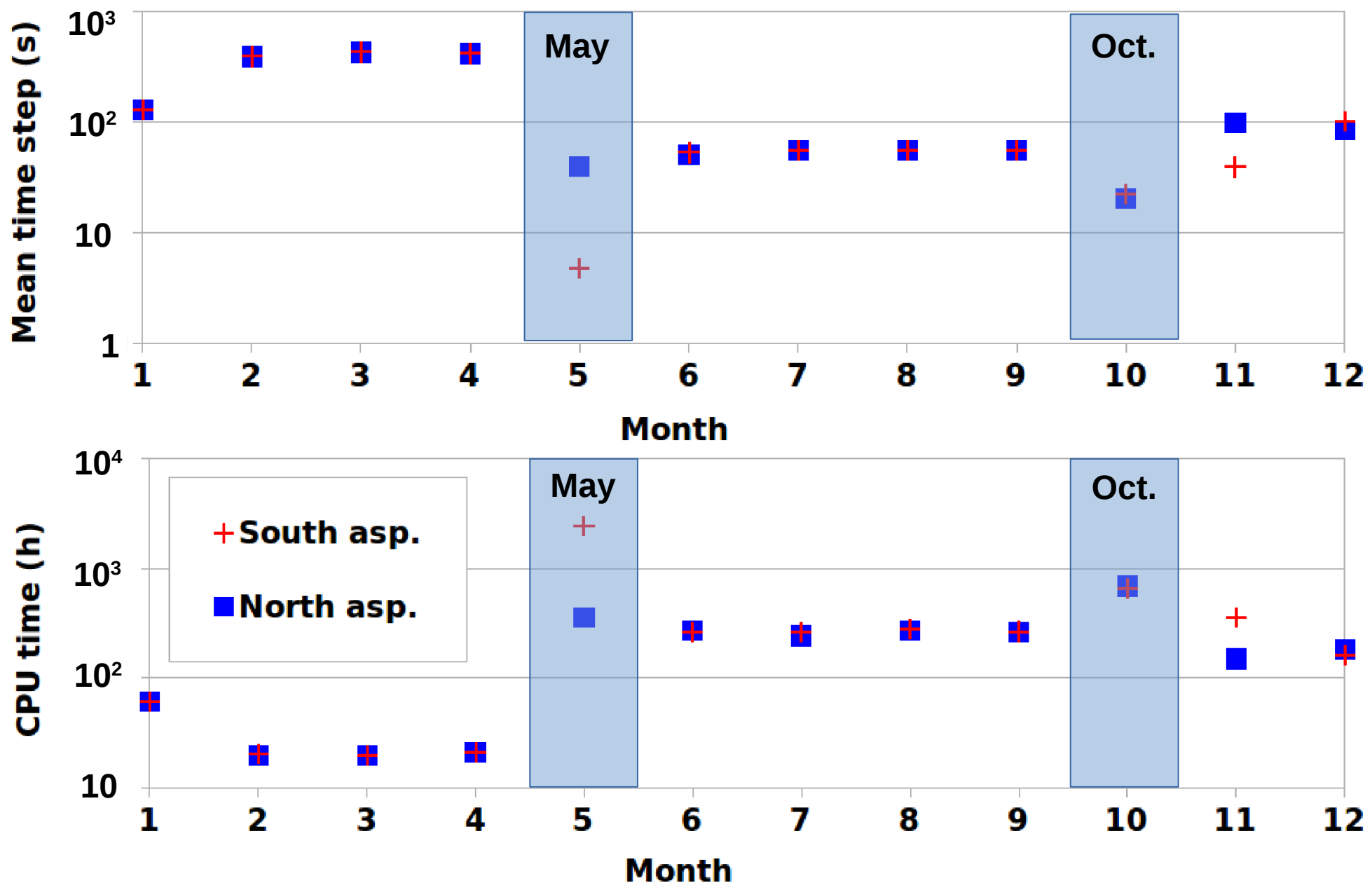


◆ AET

✕ PET

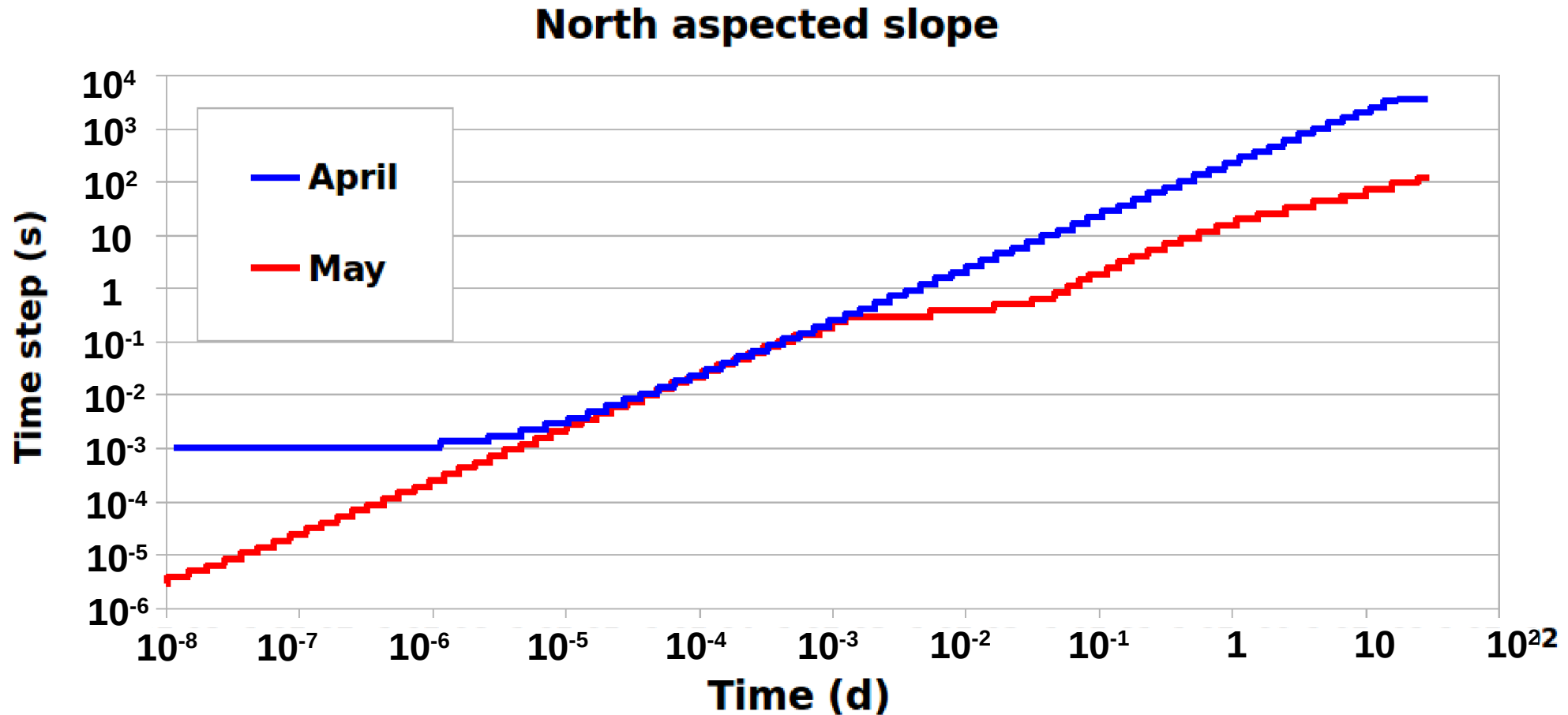
■ Rain

Numerical behaviour of computations



Periods of **transition between frozen / thawed states** are the most demanding to achieve convergence

Numerical behaviour of computations



Extremely high inter-month and intra-month **variability** of the time step !

Concluding remarks

permaFoam:

- allows to **model mechanistically permafrost dynamics** at the slope scale.
- enables to catch the first order spatial variability observed in the field (N/S slopes).
- has reasonable **parallel performances**.

Next steps

Quantification of **fluxes at the watershed scale**

Sensitivity studies

Modeling of the transfers within the moss layer

Back to the field with the understanding and issues raised from the simulation

Modeling of the permafrost dynamics in Kulingdakan under various scenarii of **climate change**

Perspectives

Produce thermo-hydrological input data for **weathering** modeling in permafrost affected catchments in boreal areas in current conditions and under climate change

Add solute transport phenomena

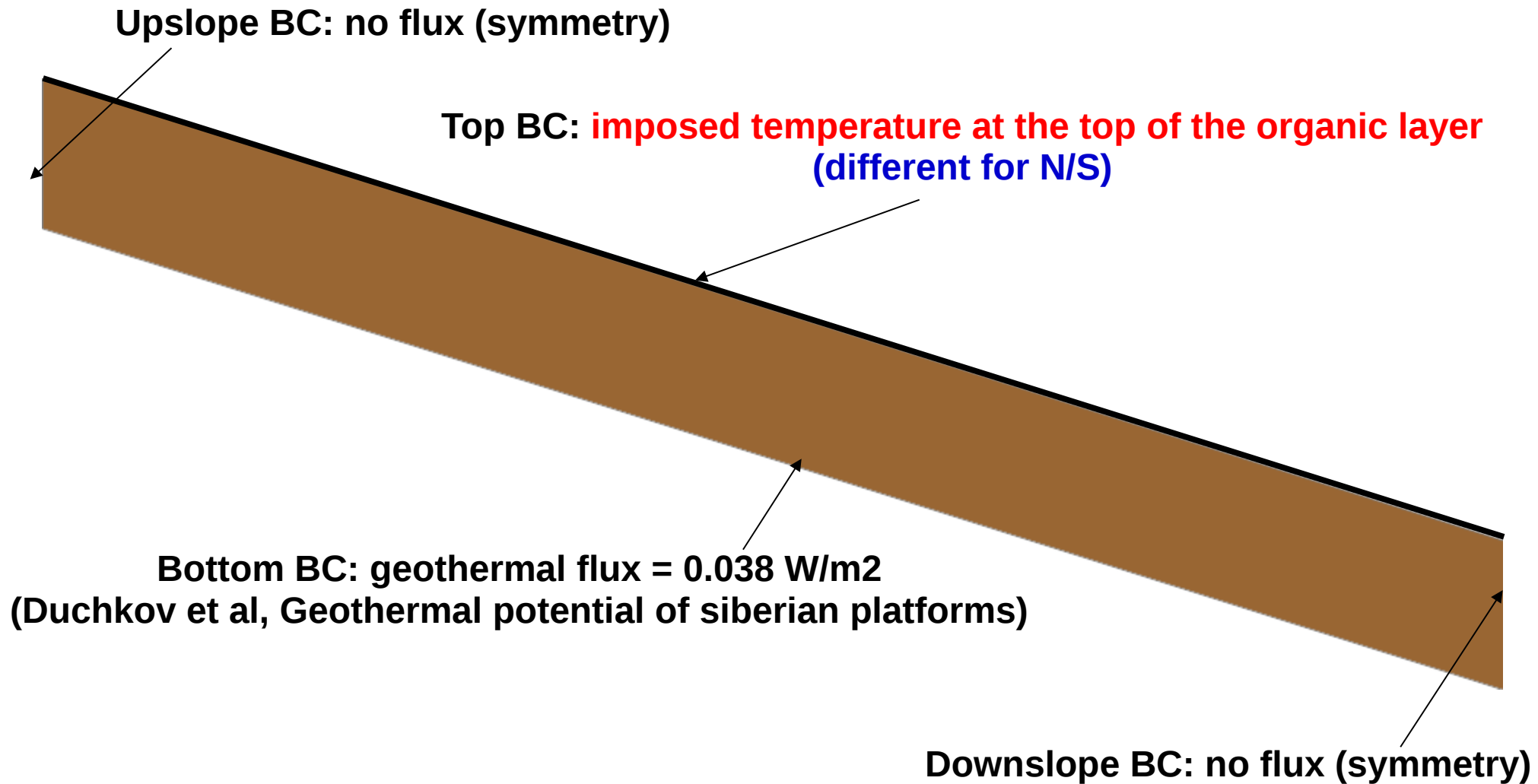
Towards more realistic modelings at the **watershed scale**: meshing DEM, pedological/geological models, taking into account soil cover heterogeneities, etc

Thank you for your attention.

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Boundary conditions for the thermal equation



Boundary conditions for the hydrological equation

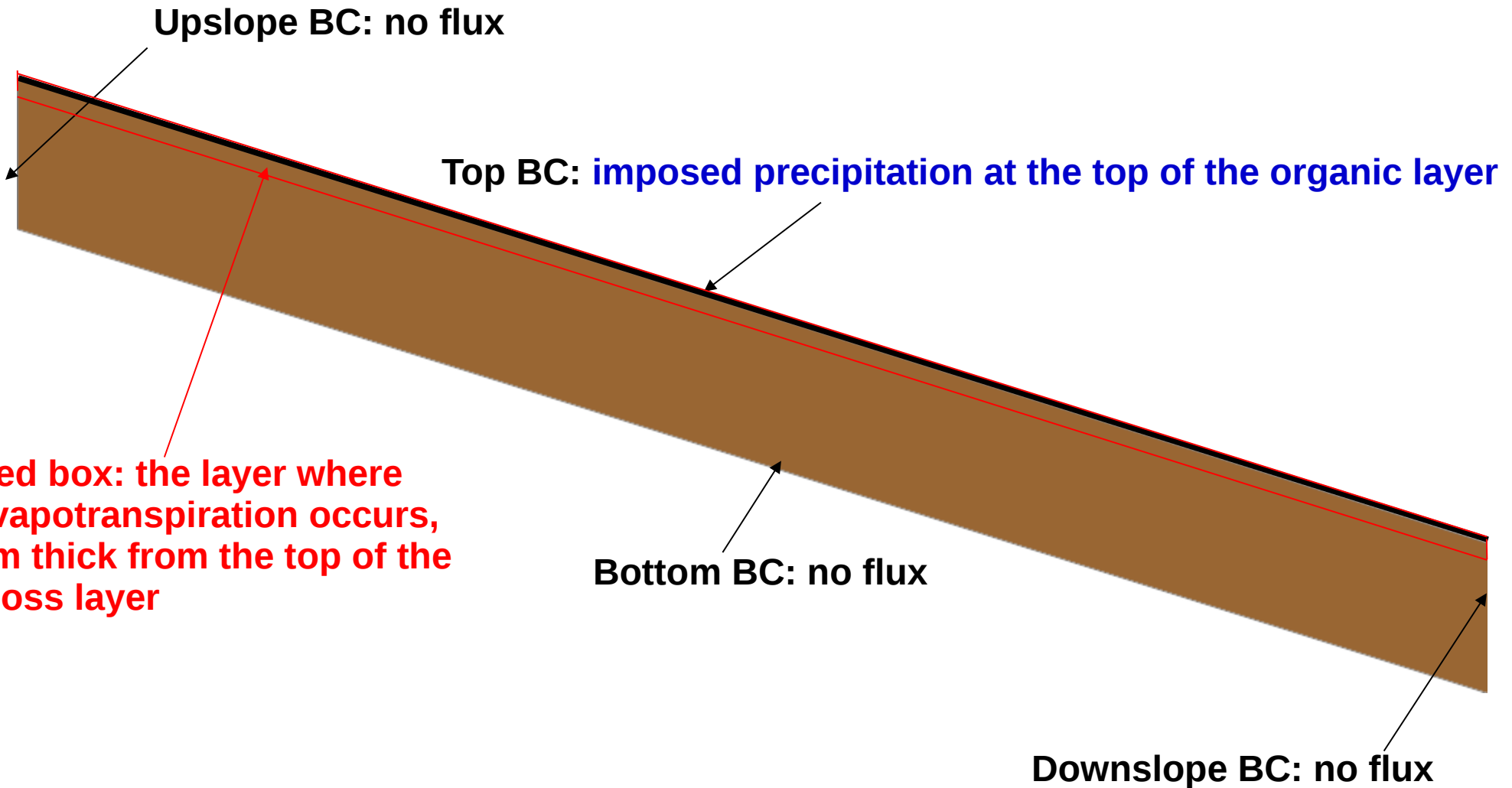
Upslope BC: no flux

Top BC: imposed precipitation at the top of the organic layer

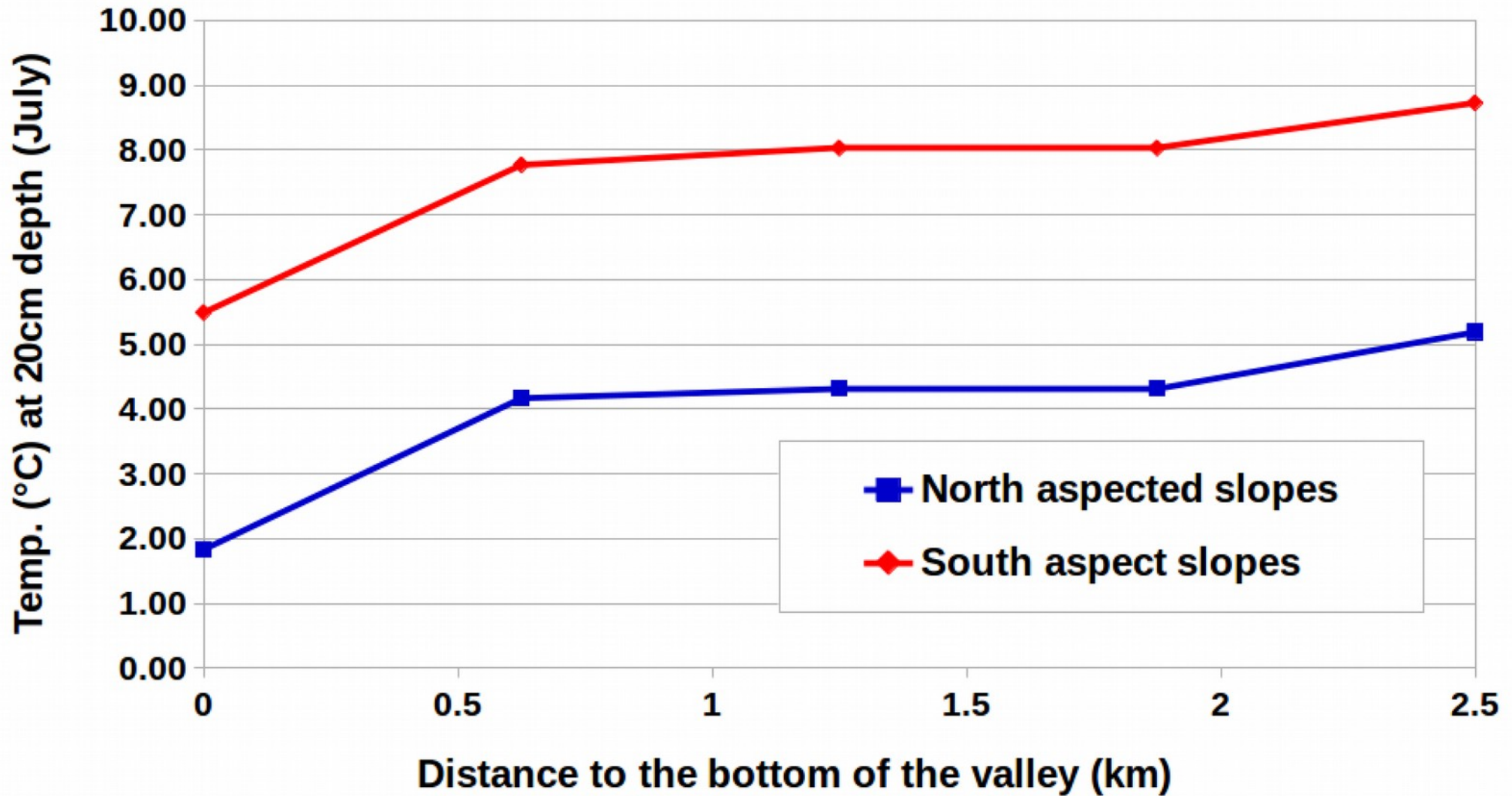
Bottom BC: no flux

Downslope BC: no flux

Red box: the layer where evapotranspiration occurs, 1m thick from the top of the moss layer



Variability along slopes



Variability along slopes is **detectable**:
hotter conditions upslope than downslope