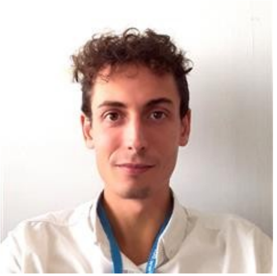
permaFoam : A parallel open-source solver for permafrost dynamics modeling

Managing parametric/century-scale simulations on supercomputers



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Université de Toulouse, France
ANR HiPerBorea - https://hiperborea.omp.eu

HiPerBorea
High Performance computing for quantifying climate change impacts on Boreal Areas

AGENCE NATIONALE DE LA RECHERCHE ANR

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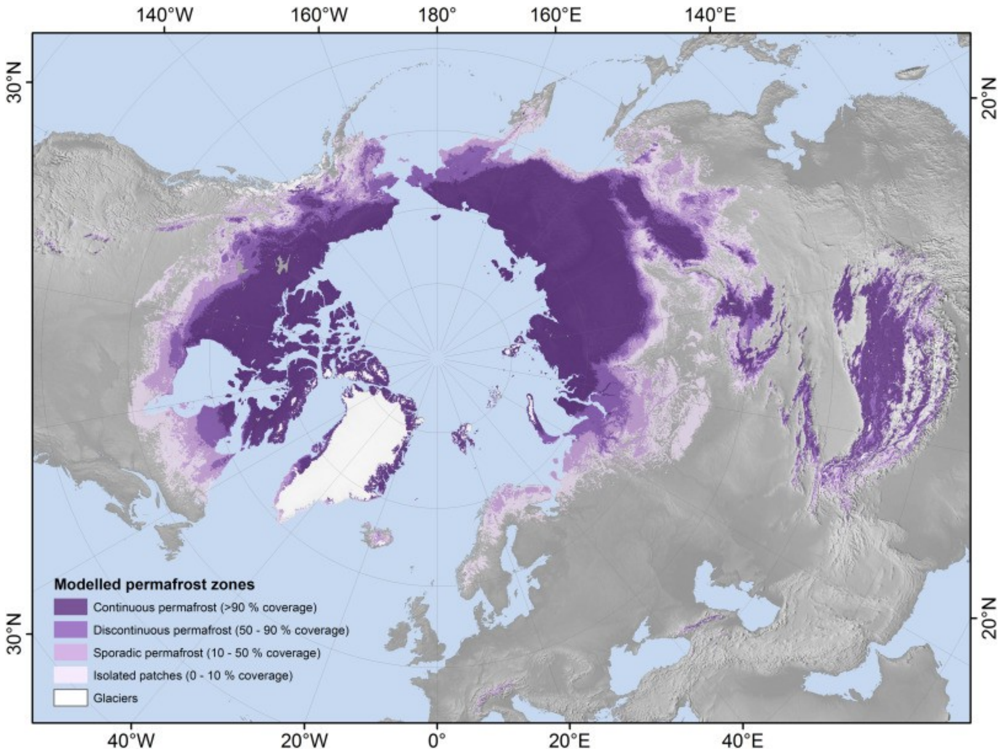
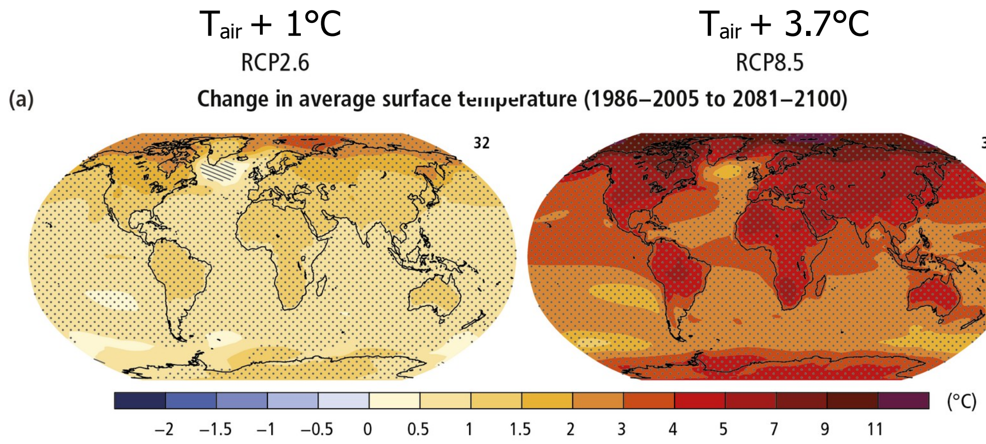
JCAD 2022

Context : permafrost under global warming



Obu et al. (2019) : Permafrost zonation based on classified modelled permafrost probabilities obtained with CRYOGRID 1.

IPCC (2014) : Inhomogeneity of temperature change in two different climate scenarios.



Permafrost
Soil layer permanently frozen
25% of northern hemisphere lands
Particularly threaten by climate change

Context : HiPerBorea project

Quantify impacts of climate change on permafrost dynamics.

Mechanistic numerical simulations for scenarios of climate change until 2100.

HiPerBorea

High Performance computing for quantifying climate change impacts on Boreal Areas

Focus on 4 experimental stations

- Abisko station, INTERACT, Sweden
- Syrdakh watershed , IRN TTS, Eastern Siberia
- Khanymey station, INTERACT, Western Siberia
- Evenkian station, INTEARCT, Central Siberia

4 partner laboratories

- Geosciences Environment Toulouse
- Institut de Mécanique des Fluides de Toulouse
- Laboratoire des Sciences du Climat et de l’Environnement
- Centre d’Etude Spatiale de la Biosphère

Support of ESI-OpenCFD for development

1 post-doc, 1 PhD, master students

Data archived and opened https://hiperborea.omp.eu/catalogue/

Introducing the code permaFoam

permaFoam : permafrost simulator

Water flow and Heat transfer with phase change
Variably saturated, variably frozen porous media
Subsurface processes (surface = BC)
Evapotranspiration
3D, Transient problems.
Heterogeneous domains

permaFoam under “hydrology” repository :
https://develop.openfoam.com/Community/hydrology

“Demo” cases to get started !

Orgogozo et al. (2019) - Orgogozo et al. (2022)

OpenFOAM®

3D Finite Volume schemes for PDE

Variety of solvers : fluid flow, heat transfer, solid mechanics, …

Maintained HPC methods.

Large community

Open-source, free for everyone

permaFoam primary equations : transfers in porous media

A - Richards equation with evapotranspiration

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

B - Heat transfer with phase change

$$\frac{\partial\left(C_T(h,T)+L\frac{\partial\theta_{ice}(h,T)}{\partial T}T\right)}{\partial t}+\nabla.\left(\boldsymbol{V}(h,T)C_{T,liquid}T\right)=\nabla.\left(K_T(h,T)\nabla T\right)$$

h : Generalized water pressure head
C_H : Capillary capacity
K_H : Apparent hydraulic conductivity
Q_{AET} : Actual evapotranspiration

T : Temperature
C_T : Equivalent heat capacity
L : vol. latent heat of fusion of ice
V : Darcy velocity
θ_{ice} : vol. frozen water content
K_T : equivalent thermal conductivity

Non-linear
Strongly coupled

OpenFOAM as development framework for permaFoam

Developing within OpenFOAM
(Core in C++)

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

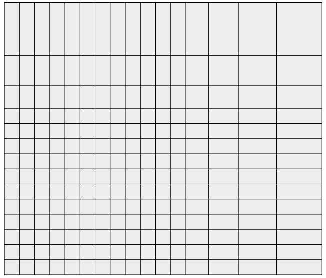
```
// Resolution of the linear system.

        // Equation (1) in reference [1]
        {
          fvScalarMatrix psiEqn
          (
            Crel*fvm::ddt(psi)
           == fvm::laplacian(Krel, psi, "laplacian(Krel,psi)")
            + gradkz
            - AET
          );
          psiEqn.solve();
        }
```

OpenFOAM as development framework for permaFoam

Run OpenFOAM in parallel...

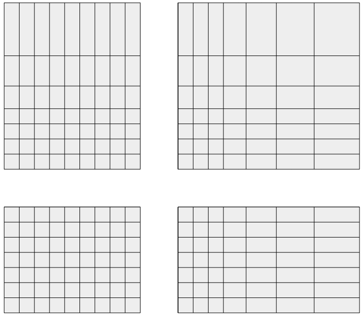
serial step
parallel step

Mesh generation



blockMesh
snappyHexMesh

1 rep. / MPI process



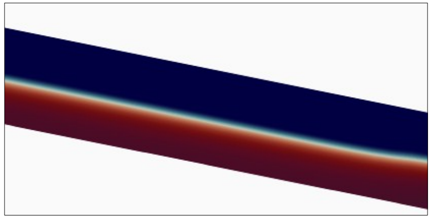
decomposePar
reconstructPar

Run & Data output

t=0...
t=1... <= Output
....
t=n... <= Output

application

Post-processing



Paraview, scripts, ...

To supercomputers… !

Supercomputer OLYMPE
CALMIP

Regional (Tier 2) - 16 464 cores
Intel© Skylake 61140
36 cores/node

…

Supercomputer OCCIGEN
CINES

National (Tier 1)
Haswell partition :
50 544 cores | 24 cores/node

…

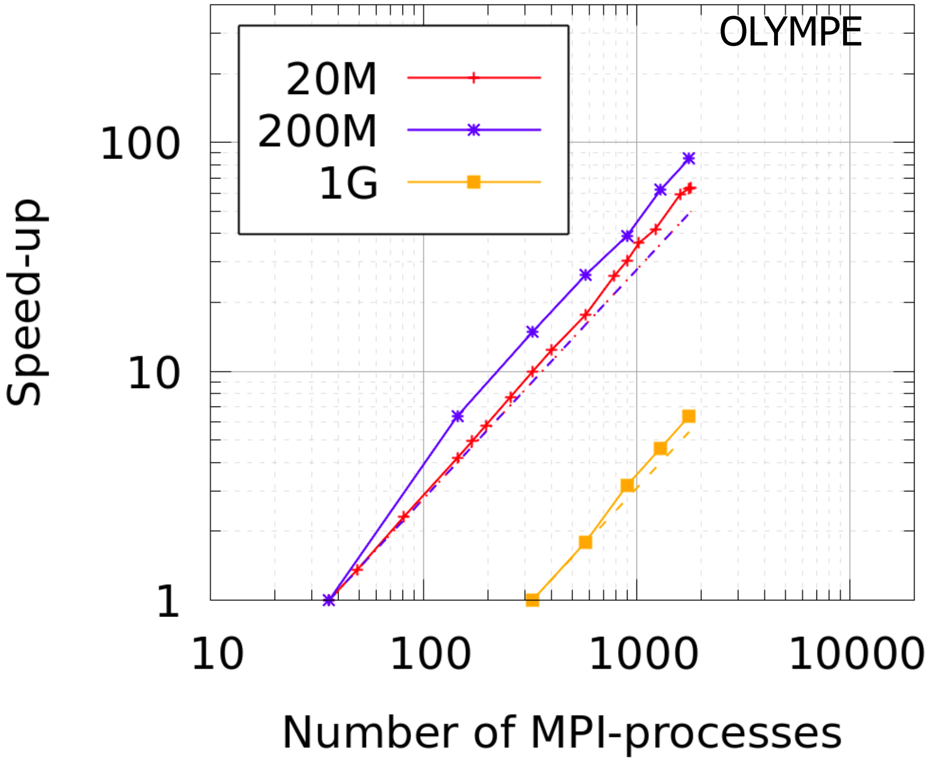
Supercomputer Joliot – Curie
TGCC

National/European (Tier 1- Tier 0)
AMD partition : 293 376 cores
AMD© Rome epyc
128 cores/node

…

Parallel performances of permaFoam

permaFoam democase (during freezing process) on different supercomputers (Tier 2 – Tier 1+) and different meshes



Parallel performances of permaFoam

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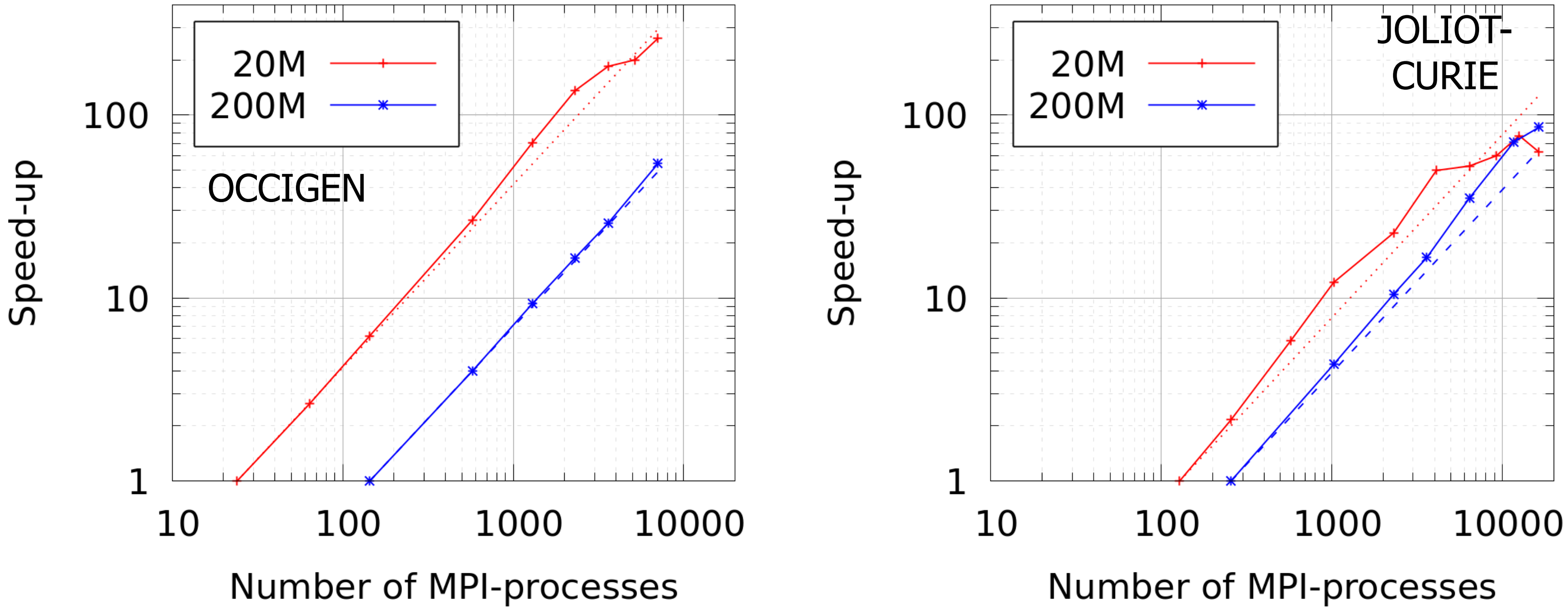


Super-linear scalability up to 16 384 cores on Joliot-Curie (AMD) with a 200 millions cells mesh

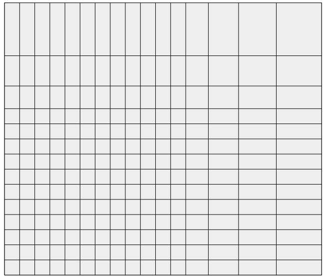
=> 7 millions hours.cpu granted to HiPerBorea by GENCI (May 2022 - April 2023)

decomposePar bottleneck for scalability study

Previously...

serial step
parallel step

Mesh generation



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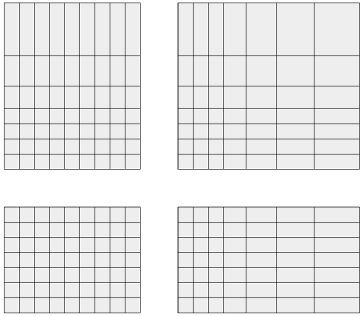
snappyHexMesh

1 rep. / MPI process



decomposePar
reconstructPar

Run & Data output

t=0...
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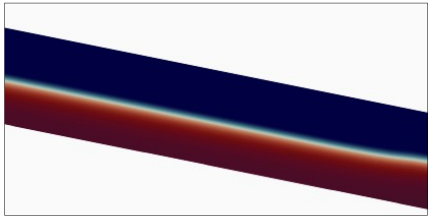
Post-processing



Paraview, scripts, ...

decomposePar bottleneck for scalability study

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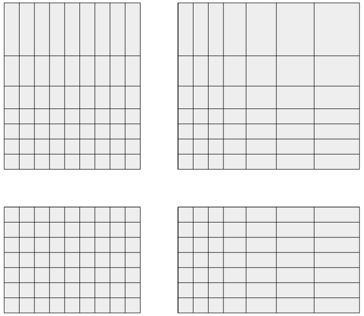

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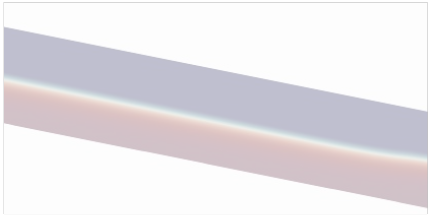


Paraview, scripts, ...

decomposePar bottleneck for scalability study

Example : decomposePar of 200M case on 16384 cores :

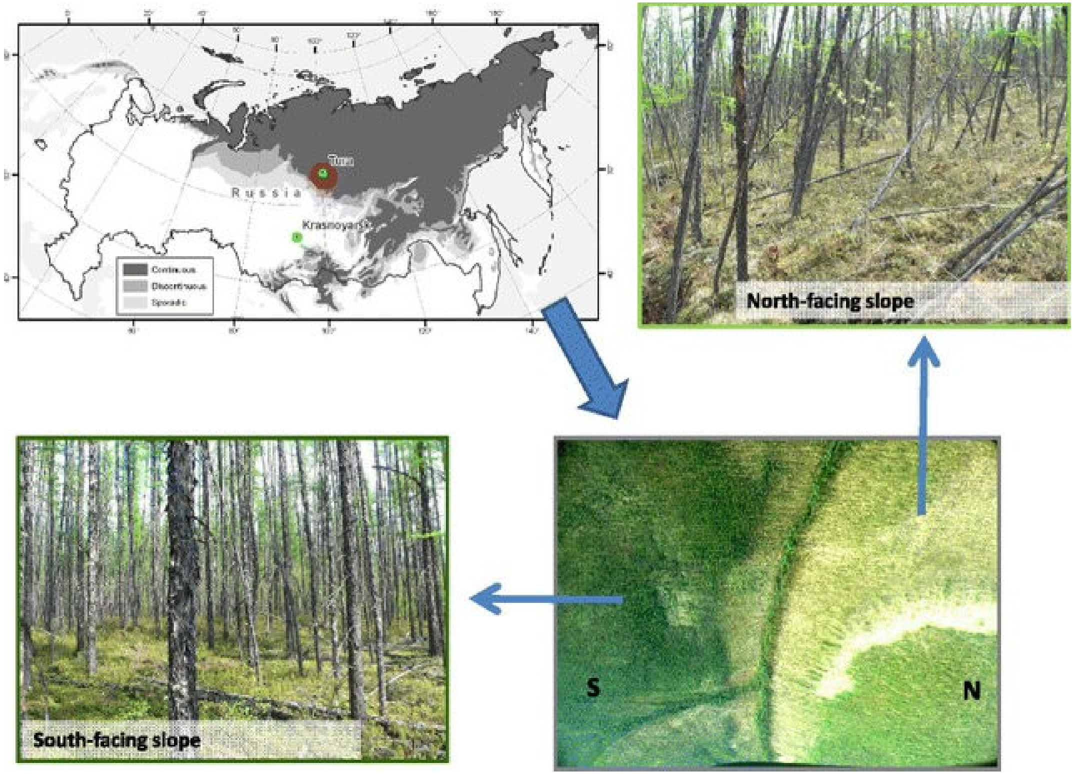
60h-150h (depending on processor) | **655k inodes** -
1G mesh cells case ~ 500Go

Problem studied during our participation to Summer of HPC 2022 (PRACE)

=> 1st version of decomposePar parallel
=> Still some sequential operations
=> Still a bottleneck (CPUTime, Memory usage)
=> New approach under investigation

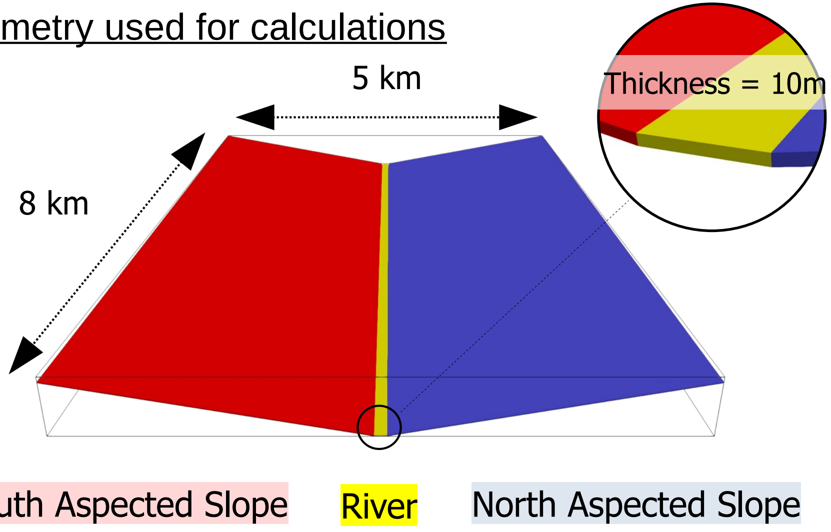
https://summerofhpc.prace-ri.eu/author/dogukant/

Application to Kulingdakan Watershed (Central Siberia)



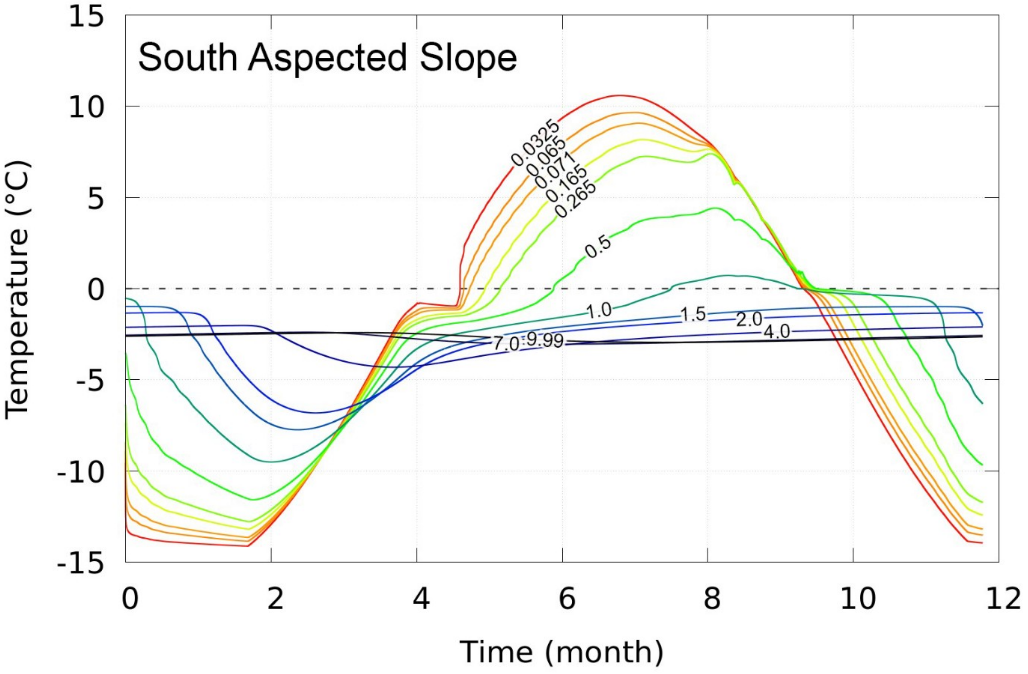
Adapted from Viers et al. (2015), Brown et al. (1981)

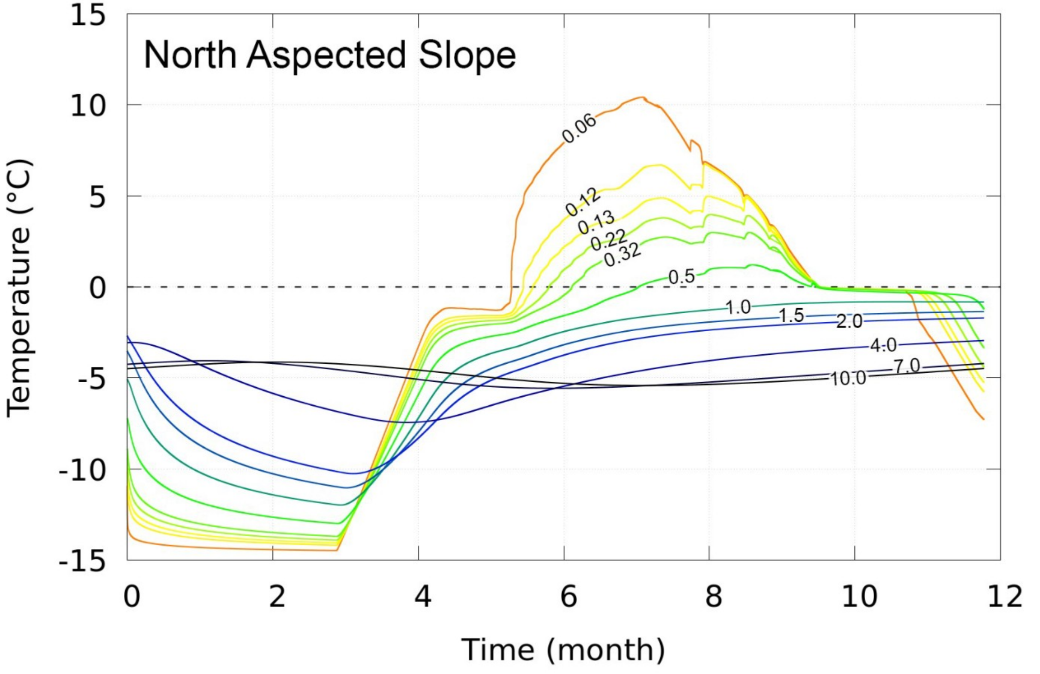
Geometry used for calculations



- North/South patches.
  - Litter properties; rooting depth
  - Unsteady boundary conditions.
- Mesh refinement close to the surface.
- Different meshes up to 500M.

Application to Kulingdakan Watershed (Central Siberia) – 3D Results



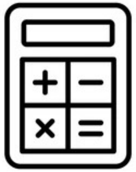


Simulation under current conditions - Good agreement to the observations (Orgogozo et al. 2022)
~48h execution time on 4000 cores. 57M mesh cells

Managing a "large" 2D parametric study

Need for 2D parametric study to explore water transfer influence on permafrost dynamics.

4 variables identified : litter and mineral soil conductivity, water transfer around freezing point
3 values for each parameters 5 years-long calculation 4 iterations saved by year
Calculation on 512 cores. 36 files / proc / iteration

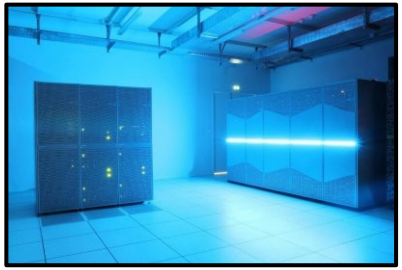


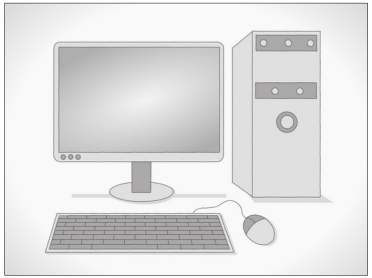
3^4 = 81 calculations
81 x 5 x 4 = 1620 iterations saved
1620 x 512 x 36 = **30M inodes**
~6 To of data expected

==> How to efficiently manage (follow+post-treat) these calculations ?

Managing a "large" 2D parametric study

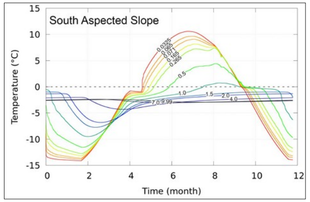
Before :





Paraview GUI
Libreoffice Calc

(Python/gnuplot)
...



Or launch calculation again...

Transfer speed
(size, inode)

RAM limitation
CPU time

Need hours
Crashes

"Large calculation" = calculation large enough to require changes in our methodology

Managing a “large” 2D parametric study

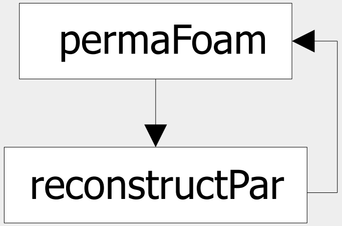
Strategy applied

Calculation Management

Formatting !

Bash script to check code logs

Automate calculation relaunch



Managing a “large” 2D parametric study

Strategy applied

#Name	LastTime(s)	LastTime(day)	LastTime(year)	number_core	TotExecutionTime(s)	TotExecutionTime(h)	HCPU	STATUT
1111	3627372	41	0	512	71773.5	19	10207	NOT_IN_QUEUE
1112	94608000	1095	3	512	202025.7	56	28732	NOT_IN_QUEUE
1113	94608000	1095	3	512	121596.9	33	17293	NOT_IN_QUEUE
1121	3615137	41	0	512	71775.8	19	10208	NOT_IN_QUEUE
1122	94608000	1095	3	512	202718.6	56	28831	NOT_IN_QUEUE
1123	94608000	1095	3	512	128290.2	35	18245	NOT_IN_QUEUE
1131	3611027	41	0	512	71802.4	19	10211	NOT_IN_QUEUE
1132	94608000	1095	3	512	203275.7	56	28910	NOT_IN_QUEUE
1133	94608000	1095	3	512	129005.4	35	18347	NOT_IN_QUEUE

Managing a “large” 2D parametric study

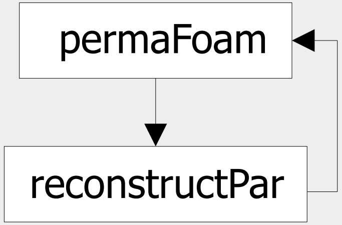
Strategy applied : formatting is a key

Calculation Management

Formatting !

Bash script to check code logs

Automate calculation relaunch



Paraview operation

On calculation nodes
No data repatriation

Python script + pvbatch

See basic presentation :
https://youtu.be/pem4QSVUGmA

Other post-treatment

Exploiting OpenFOAM probes
+ bash scripting

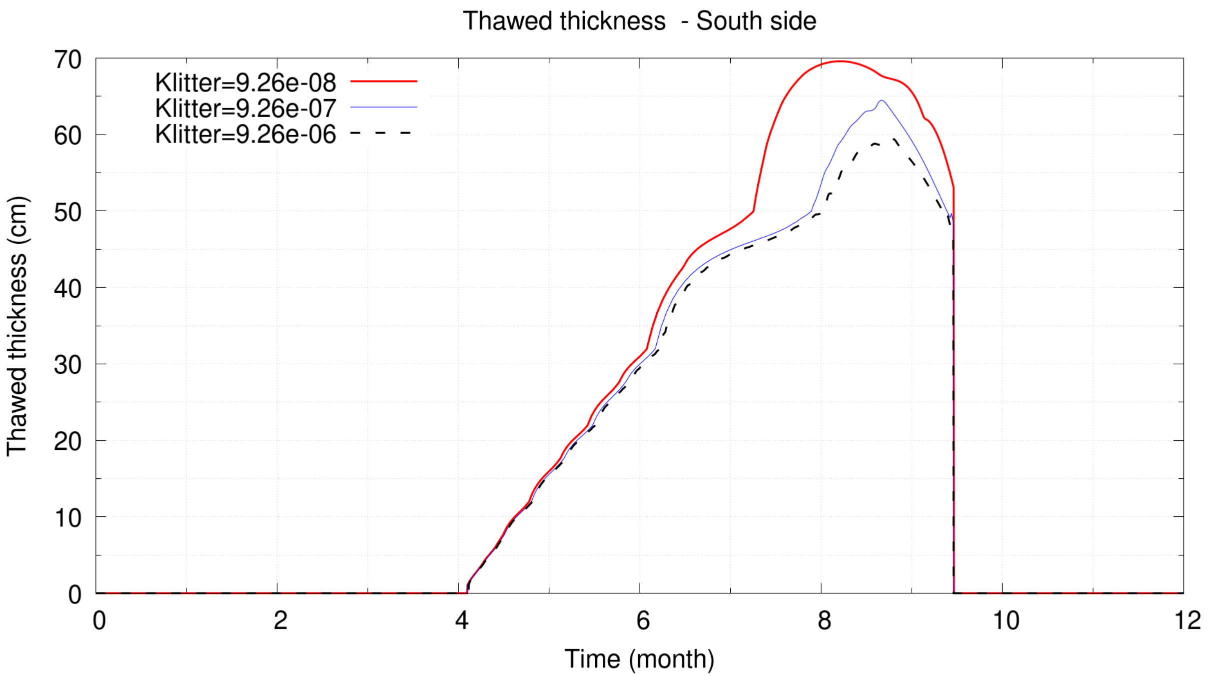
FORTRAN90 or C++ code
to read / filter /analyse large files
GNUPLOT scripts to generate PNG

No need for In-Situ or
MPI post-processing codes (yet)

One job for each calculation repertory
(SLURM scripts generation automated from models)

Managing a “large” 2D parametric study

Results : 2To of data, ~1,5M h.cpu in a few days… → Under (human) analysis



Are lateral water fluxes and related convective heat fluxes important for permafrost dynamics ?

Still a debated question !

Sjöberg, et al (2016) : yes
Kurylyk et al. (2016) : yes
Lamontagne-Hallé et al. (2018) : yes

Gao and Coon (2022) : no (under discussion)

Xavier et al…. (in prep) : **to be continued…**

Conclusion and perspectives

permaFoam free for your toolbox to simulate subsurface phenomena !

- Richards and Energy equations
- Variably saturated, variably frozen, heterogeneous
- Massively parallel
- More to come…

7M h.cpu allocation : enhanced a **renew of our methodologies**

Now conducting/analyzing on Kulingdakan watershed (Central Siberia) :

- Parametric study on mesh and physical parameters influences
- **100-years long simulation to anticipate climate change** effect on permafrost dynamics

Thank you for your attention !

Project link : https://hiperborea.omp.eu

PermaFoam : https://develop.openfoam.com/Community/hydrology

Thibault XAVIER[1], Laurent Orgogozo[1]

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HiPerBorea

High Performance computing for quantifying climate change impacts on Boreal Areas

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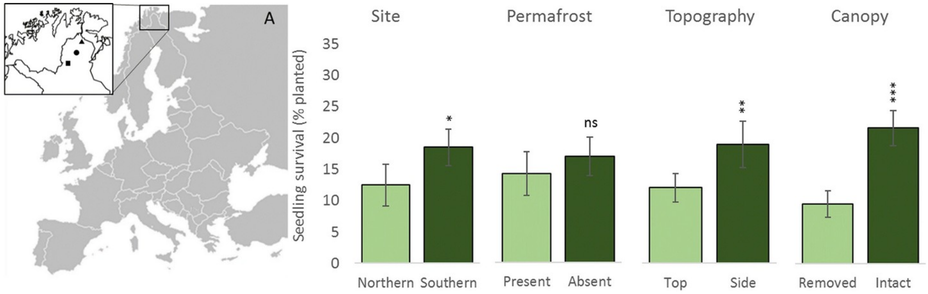
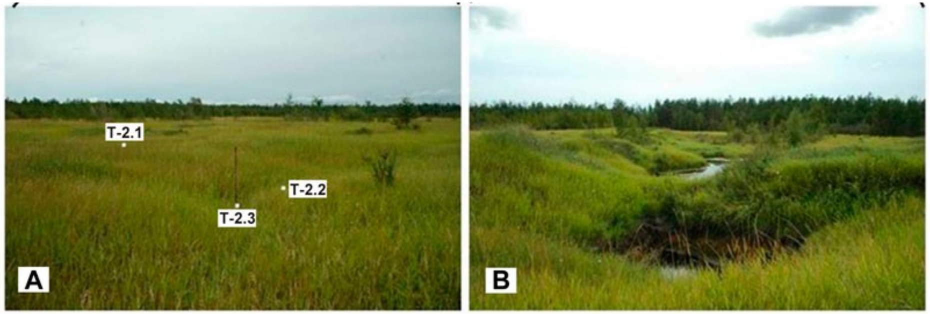
JCAD 2022

Permafrost thawing impacts

US Army Corps of Engineers (2017)
Thule Air Force base in Northwest Greenland experiences damages from permafrost thaw.



Limens et al (2021)
"Shrubs and Degraded Permafrost Pave the Way for Tree Establishment in Subarctic Peatlands" - Finnish Lapland



Desyatkin et al. (2021)
Thermokarst on former flat arable land in Eastern Siberia

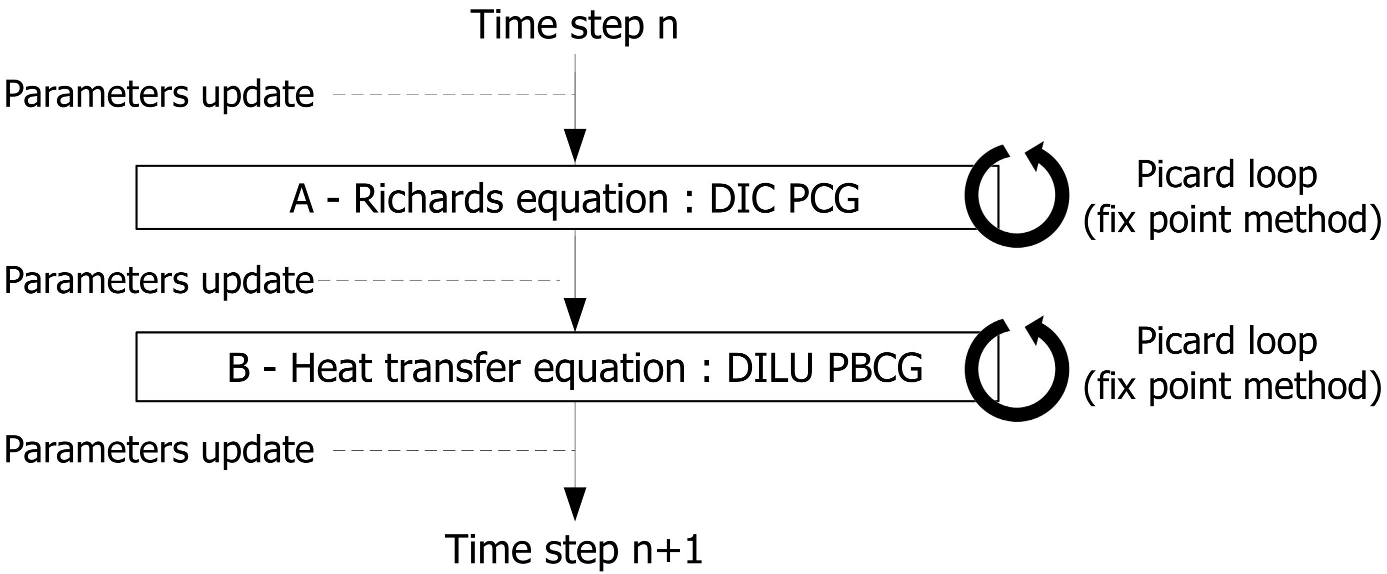
Permafrost thawing is detected at all longitudes

Many consequences : local ecology, climate change feedback, new trade routes, changes in arable lands, access to underground resources ...

Numerical framework of permaFoam.

Temporal scheme

Backward Euler time stepping
Adaptive Δt

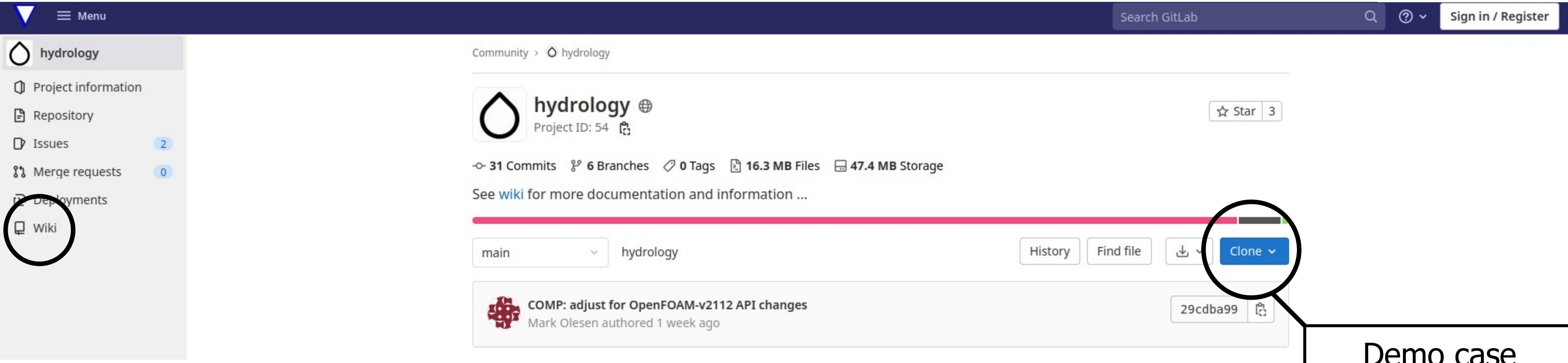


Validated in Interfrost benchmark (13 codes) – Grenier et al (2018.)

permaFoam included in open-source "hydrology" package

https://develop.openfoam.com/Community/hydrology

Or on your search engine "OpenFoam hydrology" "OpenFoam permafrost"



Demo case included to get started !

New users, feedbacks, contributions ... are welcomed !

Try during Summer of HPC 2022

1 Week training by PRACE+7 weeks project

=> Discover HPC methods and environment
=> Top-students from all Europe
=> In-situ or remote project
=> Funded by PRACE

Dogukan Teber (Turkey)

Stavros Dimou (Greece)

https://summerofhpc.prace-ri.eu/author/dogukant/

Creation of a partially parallel version of decomposePar
Better performances (x2)… but still a bottleneck (memory usage, CPU time)

New methodology under investigation...

Application to Syrdakh study site (Eastern Siberia) - WIP

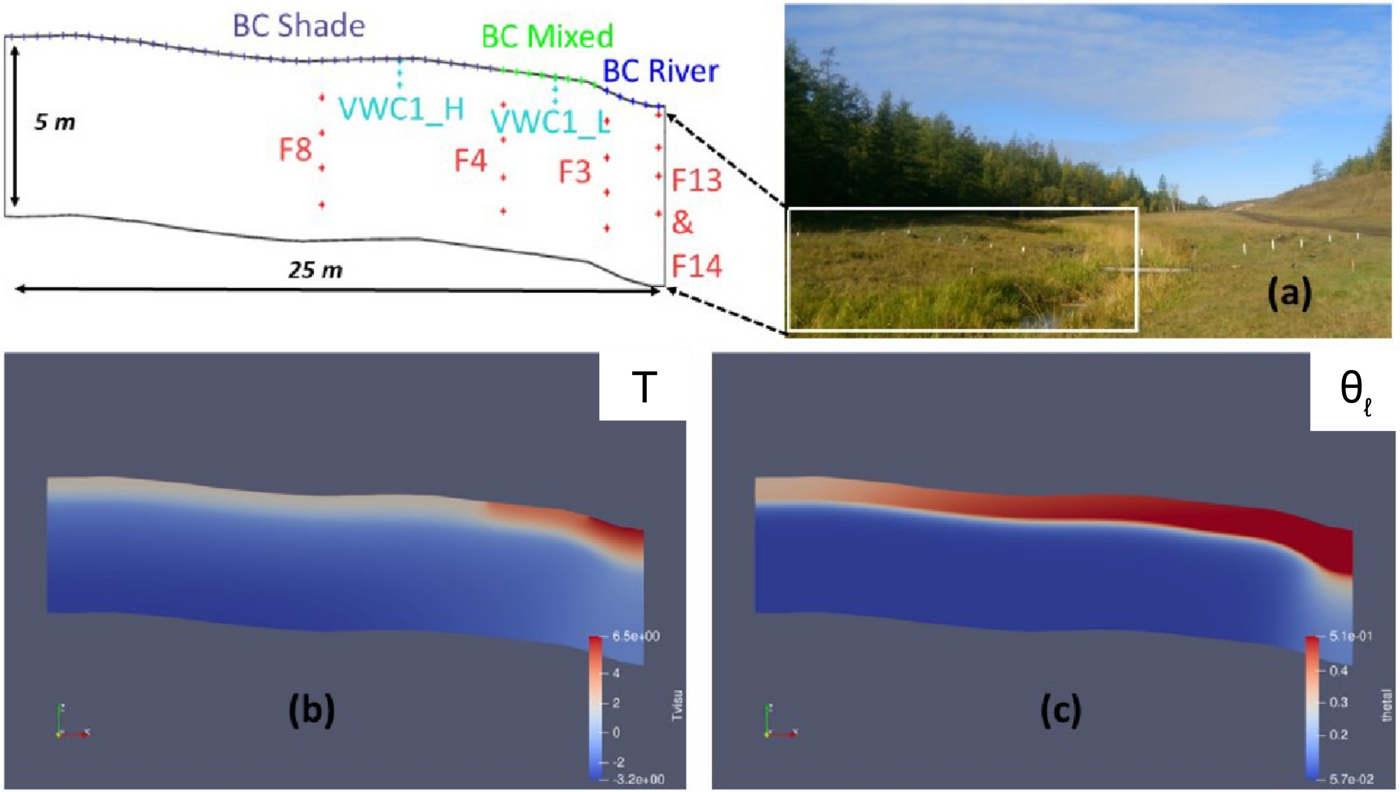
~100 km NE of Yakutsk in Central Yakutia (Eastern Siberia)

Permafrost river interaction

Instrumented cross section to a river (2012)

25m x 5m

Thermal and Hydrological measurement



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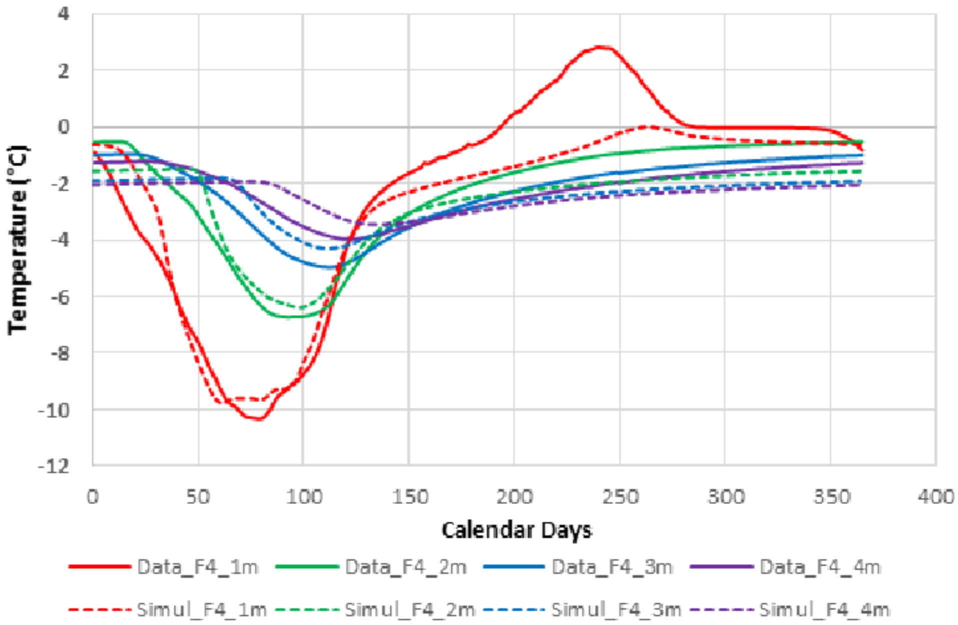
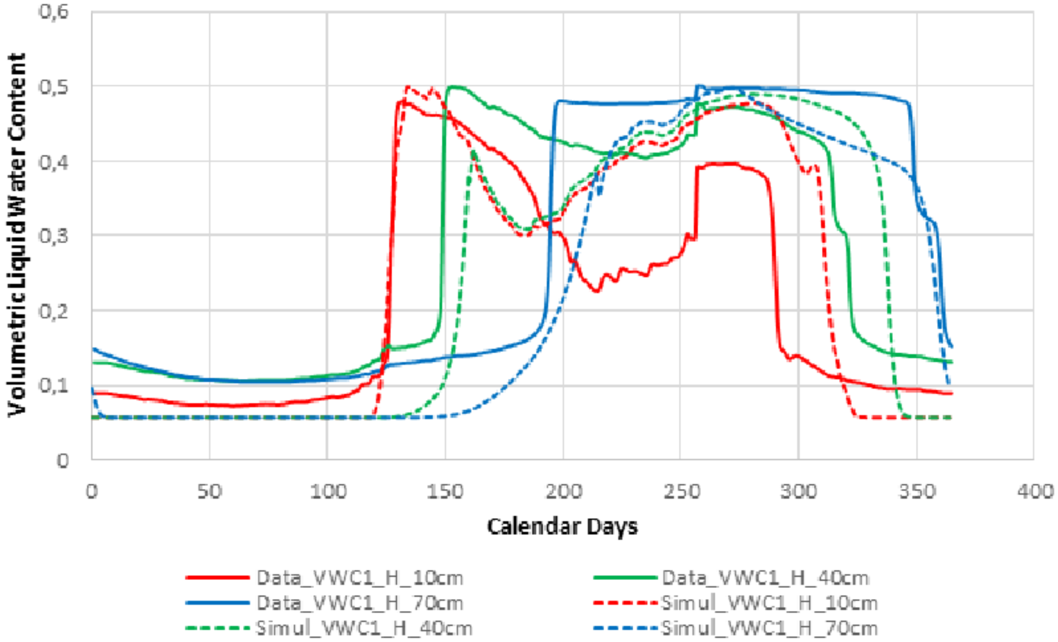
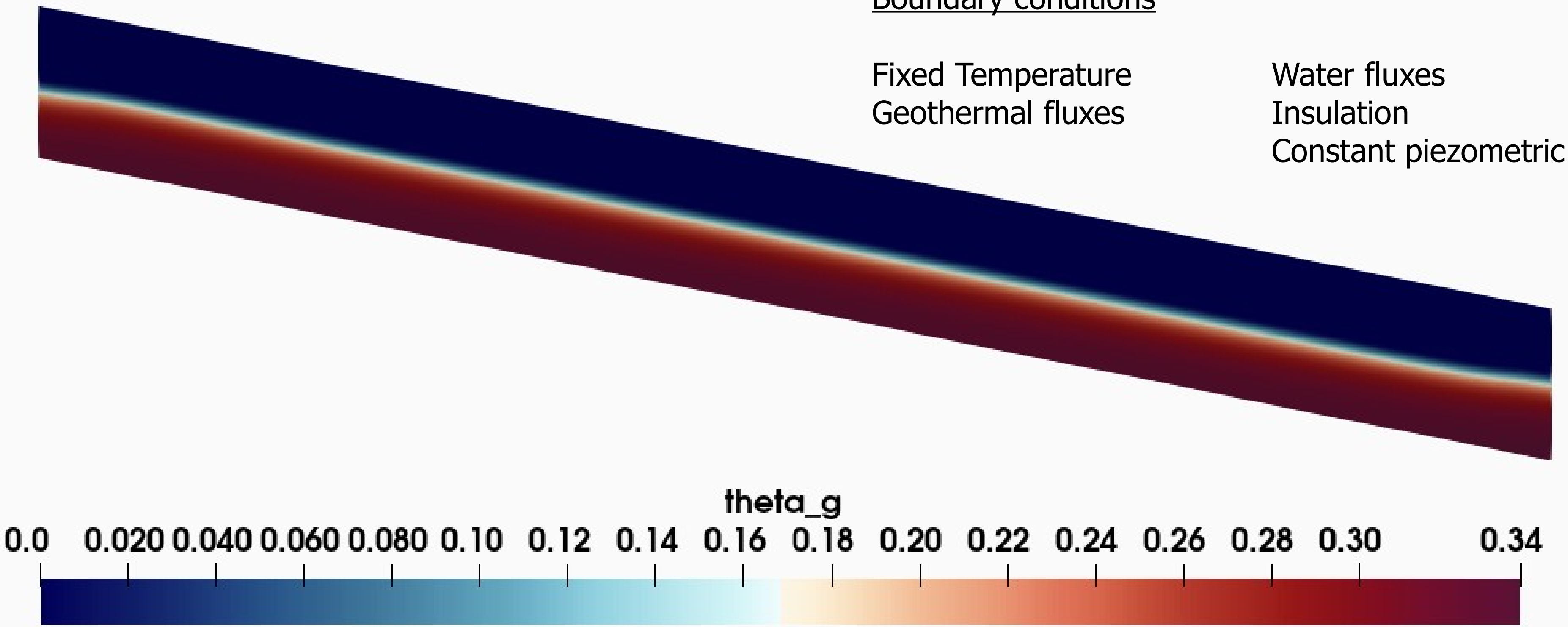




First run without calibrating soil properties to field data
Qualitative global agreement

Case example – permaFoam tutorial



Boundary conditions

Fixed Temperature
Geothermal fluxes

Water fluxes
Insulation
Constant piezometric head