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A massively parallel OpenFOAM® solver for Richards equation: Towards mechanistic modelling of transfers at the watershed scale

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Transfers of water in soils : flow in unsaturated porous media



agriculture (nitrates transfer, ...)



environnemental engineering (waste storage, ...)



earth sciences (weathering processes, ...)

Flow in unsaturated porous media : Richards equation

usual conditions of pressure and temperature, fully connected air phase:
a single equation for the unsaturated flow (Richards, 1931)

$$c(h) \frac{\partial h}{\partial t} = \text{div}(k(h) \mathbf{K} \cdot \nabla(h + z))$$

$$c, \text{ the capillary capacity } [L^{-1}], \begin{cases} c = S & \text{if } h \geq 0 \\ c = c(h) & \text{if } h < 0 \end{cases}$$

$$k, \text{ the relative permeability } [-], \begin{cases} k = 1 & \text{if } h \geq 0 \\ k = k(h) & \text{if } h < 0 \end{cases}$$

$c(h)$ ($= \partial\theta/\partial h$) and $k(h)$ functions : experimentally fitted following various models (e.g. van Genuchten 1980, Brooks and Corey 1964)

Flow in unsaturated porous media : Richards equation

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a single equation for the unsaturated flow (Richards, 1931)

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Non linearity



Mechanistic modelling at large scales ?

- (i) **Mechanistic modelling** (here, numerical resolution of 3D Richards equation) is recognized as the « **gold standard** » for the study of water transfers in hydrosystems (Miller *et al.*, 2013).
 - (ii) One of the main problems in such modelling approaches is the **large scales** that may be encountered both **in space and time** (e.g.: in the field of weathering processes study, Beaulieu *et al.*, 2012, Godd ris *et al.*, 2012).
 - (iii) These large scales imply **huge memory needs** and **long computation times**.
 - (iv) The major way to deal with such large size problems: **massively parallel computing** (e.g.: Coumou *et al.*, 2008, Hammond *et al.*, 2011, Maxwell, 2013).
- **many published softwares for Richards equation resolution** (e.g.: Ababou *et al.*, 1992, Šim nek *et al.*, 1998, 2008, Weill *et al.*, 2009), **but use of massively parallel computing is needed.**

Our approach : **RichardsFOAM**, a **massively parallel solver for Richards equation** developed in the framework of **OpenFOAM®** (e.g. Weller *et al.*, 1998, www.openfoam.com).

RichardsFOAM Validation ? Parallel performances ?

OpenFOAM® (www.openfoam.com)


The open source CFD toolbox


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12 Sep 2012: ESI Group acquires OpenCFD | [Press Release](#) | [FAQ](#)

About OpenFOAM


OpenFOAM is a free, open source CFD software package developed by [OpenCFD Ltd](#) at [ESI Group](#) and distributed by the [OpenFOAM Foundation](#). It has a large user base across most areas of engineering and science, from both commercial and academic organisations. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics. [More...](#)

Our commitment to the users

OpenFOAM comes with full commercial support from ESI-OpenCFD, including [software support](#), [contracted developments](#) and a programme of [training courses](#). These activities fund the development, maintenance and release of OpenFOAM to make it an extremely viable commercial open source product.

Our commitment to open source

ESI-OpenCFD are committed to open source software, working with the [OpenFOAM Foundation](#) to manage and distribute OpenFOAM. Through its Bylaws, it formalises the commitment, begun by OpenCFD in 2004, to ensure OpenFOAM will **always be free open source only**. ESI-OpenCFD contributes the code developments and maintenance work of OpenFOAM to the Foundation.

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News on Twitter

*A complimentary #OpenFOAM seminar day will take place in Southfield (Detroit), MI on 16 Oct 2012. For details, see <http://t.co/OwXG6TYK>
Sep 25th 2012

*Agenda released for #CFD and #OpenFOAM session at #ESI Global Forum, 18-19 October, San Diego: <http://t.co/QinecnS6>
Sep 25th 2012

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Main News

OpenFOAM Events Oct 2012
ESI-OpenCFD will showcase OpenFOAM at events in the US on 16 and 18/19 Oct 2012.
Sep 24th 2012

ESI acquires OpenCFD Ltd.
ESI-Group acquires OpenCFD, the open source leader in CFD and producer of OpenFOAM.
Sep 12th 2012

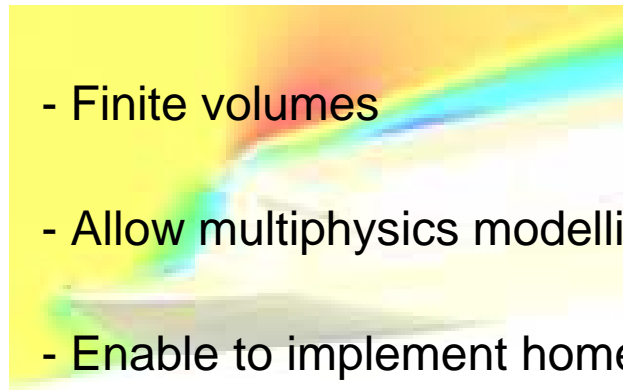
OpenFOAM Training 2013
OpenCFD is delivering OpenFOAM training courses in Jan-Mar 2013 in London, Houston, Munich, Melbourne and Shanghai.
Jul 18th 2012

[Main News Archive...](#)

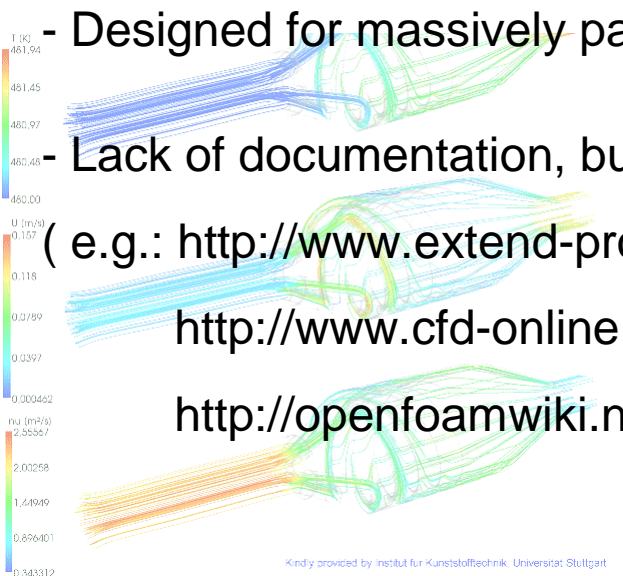
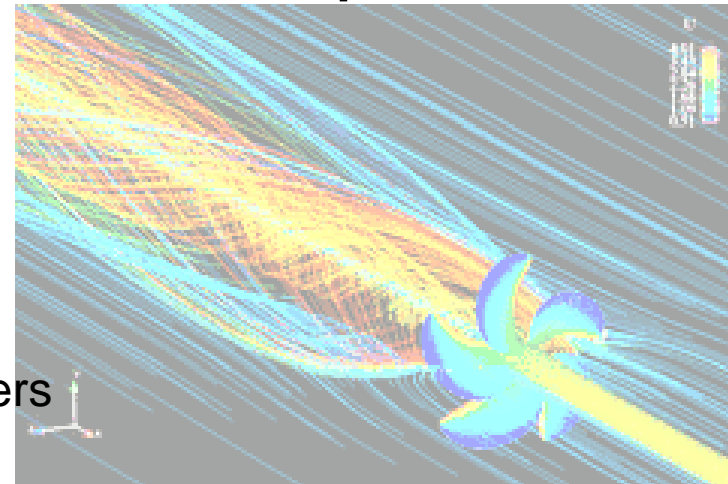
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OpenFOAM® (www.openfoam.com)

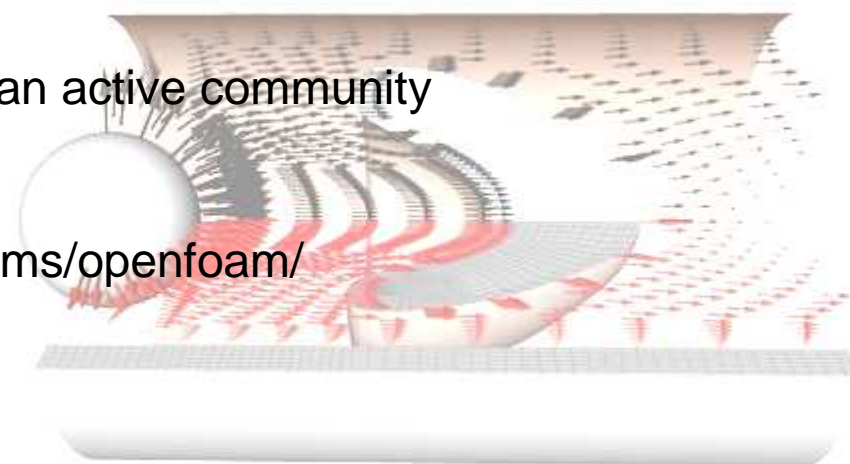
OpenFOAM® : an open source CFD tool box, developed in c++



- Finite volumes
- Allow multiphysics modelling
- Enable to implement home-made solvers



- Designed for massively parallel computing
- Lack of documentation, but there is an active community
(e.g.: <http://www.extend-project.de>
<http://www.cfd-online.com/Forums/openfoam/>
<http://openfoamwiki.net>)



Implementation of RichardsFOAM

- **Non-linearities : Picard iteration method**
- **Chord slope approximation for the capillary capacity**
- **Gravity is handled explicitly while pressure effects are handled implicitly**
- **Backward time scheme, with stabilized adaptative time step procedure**
- **Linear solver : DIC PCG**

→ RichardsFOAM

Validation: comparison with an analytical solution

Analytical validation :

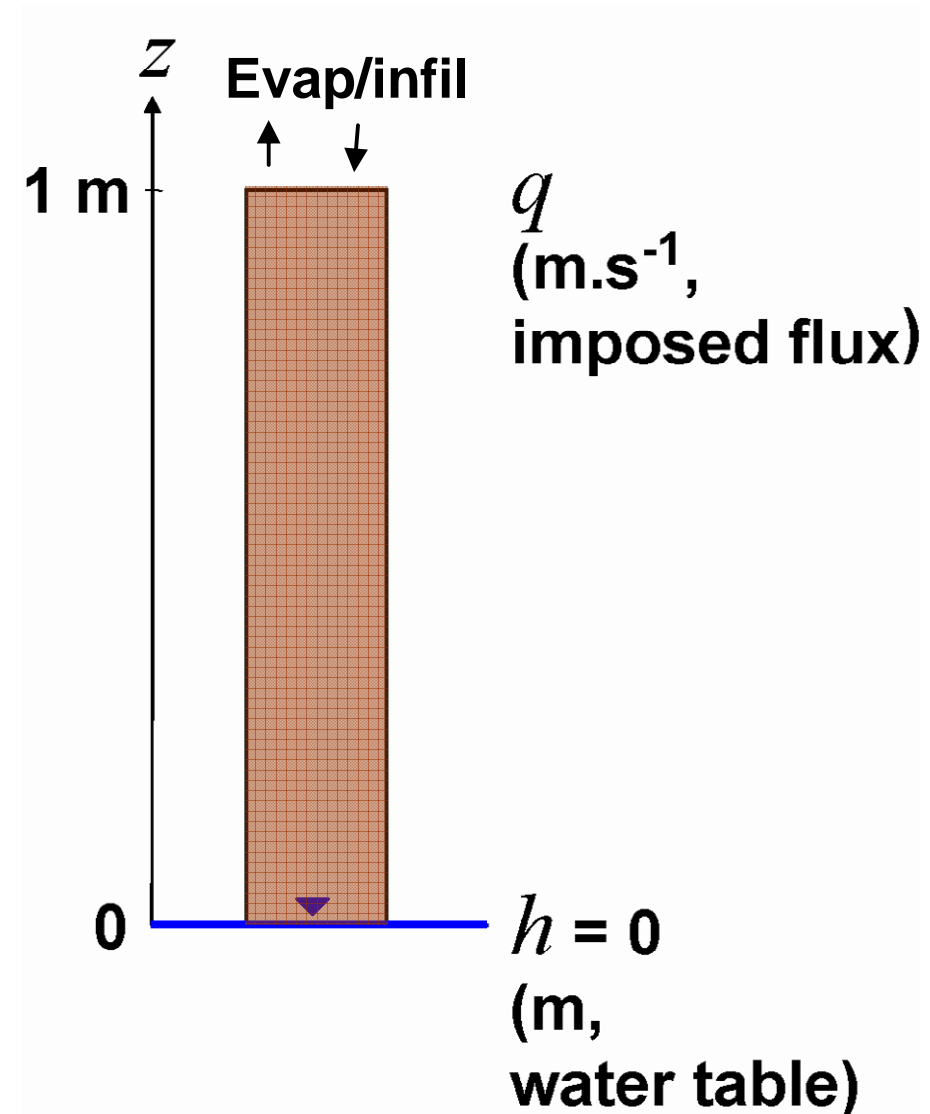
- Stationary regime
- 1D soil column
- Gardner's type permeability

One can establish an analytical solution for the configuration below.

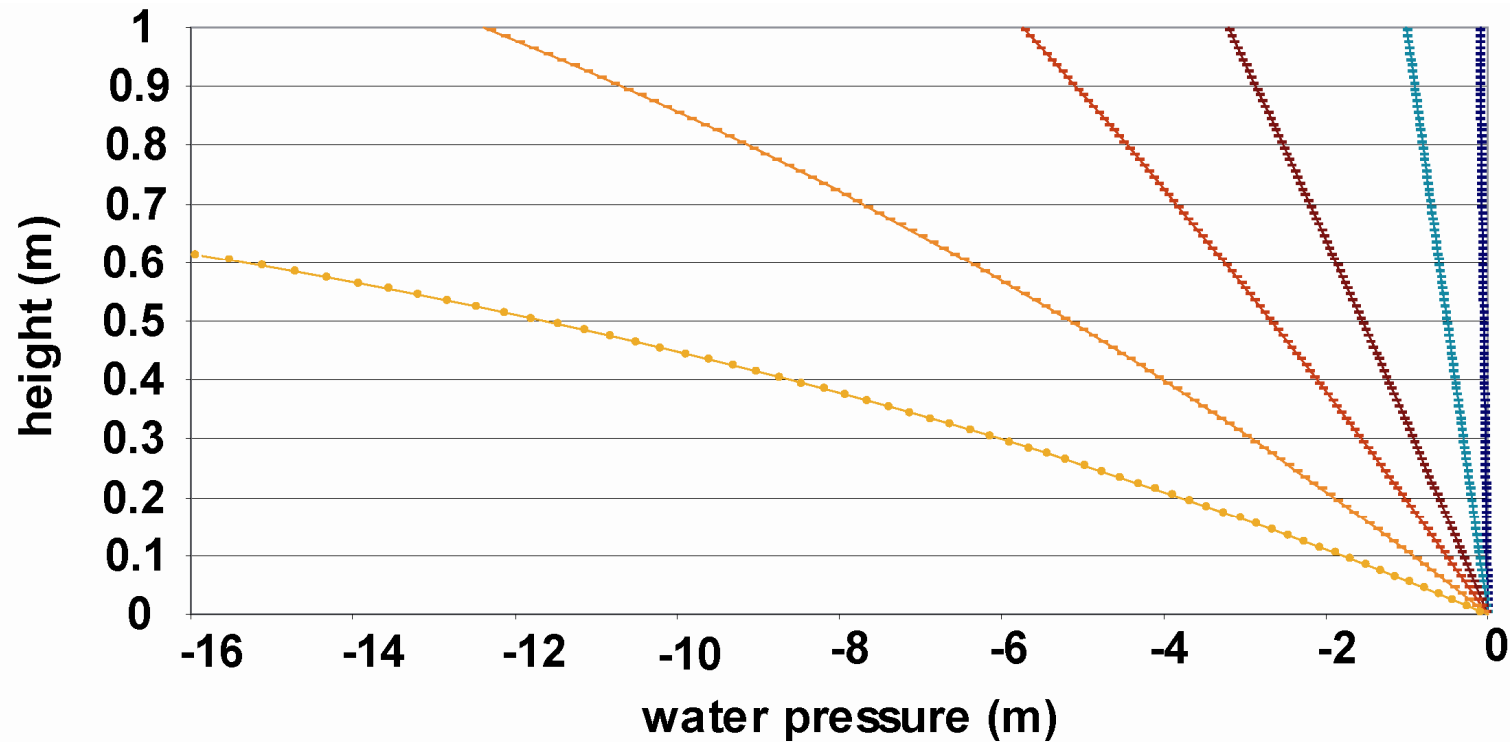
Here we consider:

$$K_{sat} = 10^{-6}$$

$$\alpha = 0,06$$



Validation: comparison with an analytical solution



— infiltration $qlK_{sat} = -0.9$
analytic

- infiltration $qlK_{sat} = -0.9$
RichardsFOAM

— evaporation $qlK_{sat} = 8$
analytic

- evaporation $qlK_{sat} = 8$
RichardsFOAM

— hydrostatic $qlK_{sat} = 0$
analytic

- hydrostatic $qlK_{sat} = 0$
RichardsFOAM

— evaporation $qlK_{sat} = 4$
analytic

- evaporation $qlK_{sat} = 4$
RichardsFOAM

— evaporation $qlK_{sat} = 2$
analytic

- evaporation $qlK_{sat} = 2$
RichardsFOAM

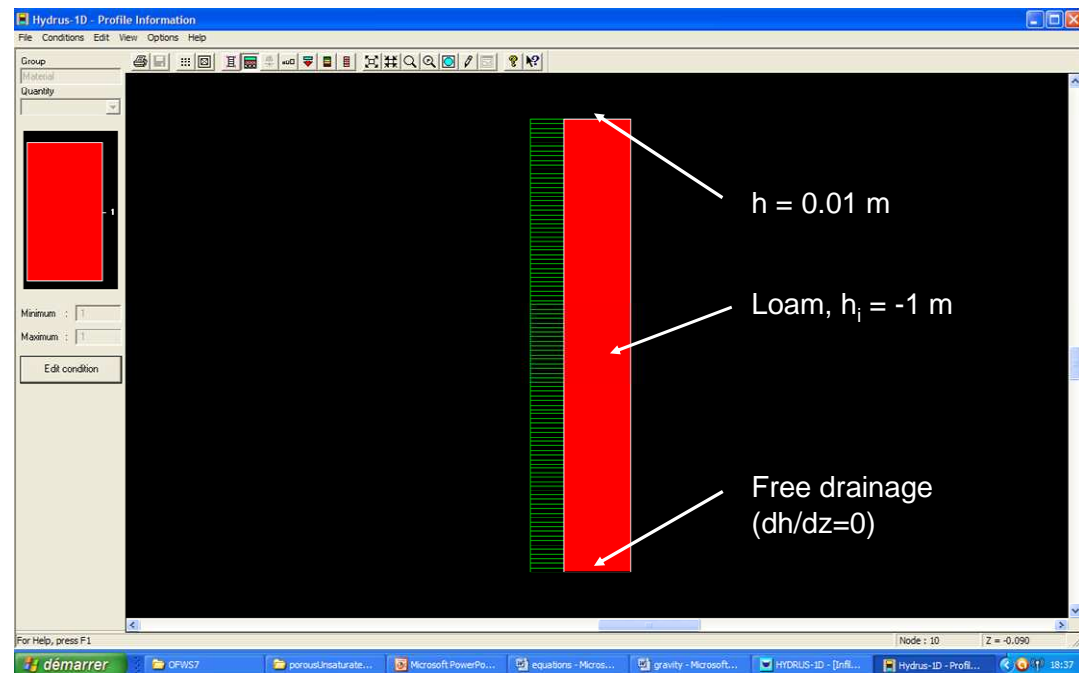
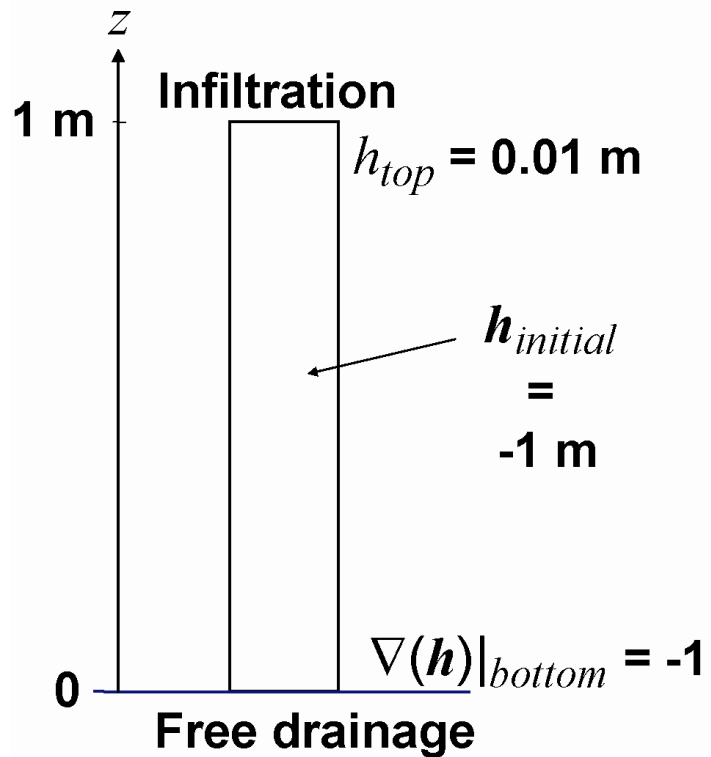
— evaporation $qlK_{sat} = 16$
analytic

- evaporation $qlK_{sat} = 16$
RichardsFOAM

➔ **Good validation in stationary regime**

Validation: comparison with Hydrus 1D (PC-Progress)

Infiltration in a loam soil column

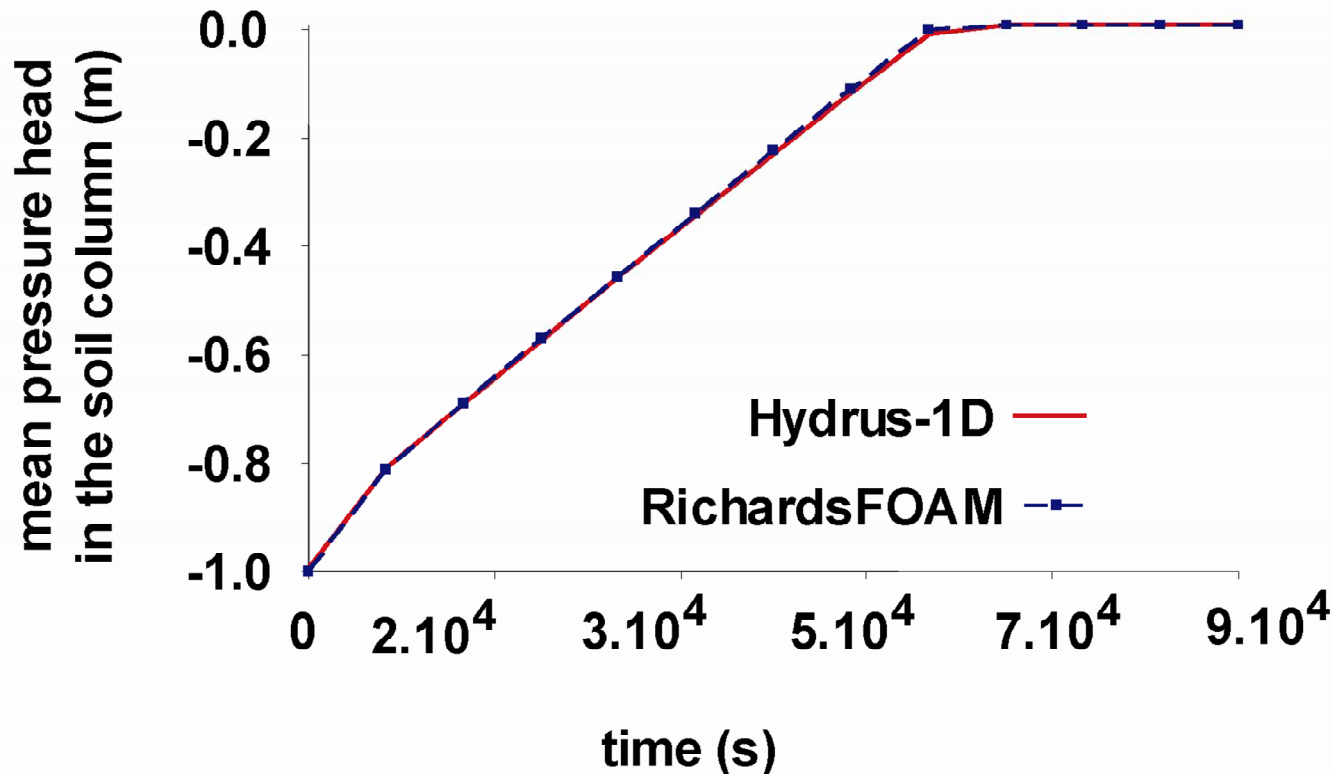


$$K_{sat} = 2.89 * 10^{-6} \text{ m.s}^{-1} \quad \alpha = 3.6 \text{ m}^{-1} \quad n = 1.56 \quad \theta_s = 0.43 \quad \theta_r = 0.078$$

(e.g.: Šimůnek et al., 1998, 2008)

Validation: comparison with Hydrus 1D (PC-Progress)

Comparison of transient results



➔ **Good agreement: difference between mean pressure heads smaller than precisions of computations (1 cm)**

(In progress : application to a field data set of south india with heterogeneous soil and monsoon climate)

Parallel performances : strong and weak scalings

How does the code behave when used on hundreds to a thousand of cores ?

Parallel acceleration: strong scaling (same problem, more and more processors) from 16 to 1024 cores

Sizing behaviour: weak scaling (bigger and bigger problem as well as more and more processors) from 16 to 1024 cores

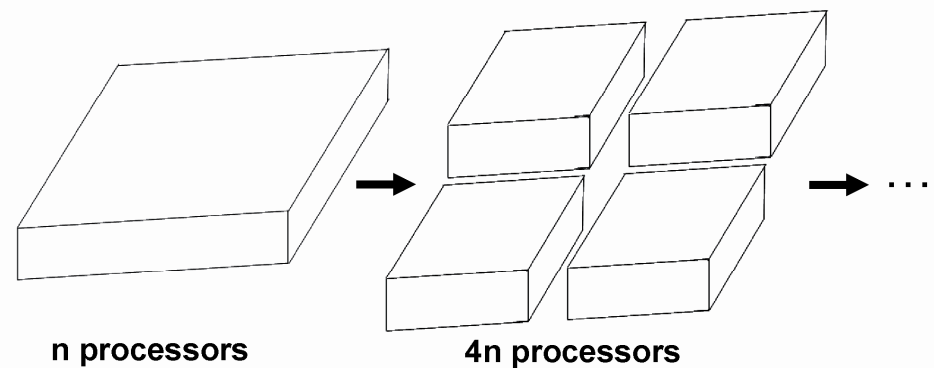
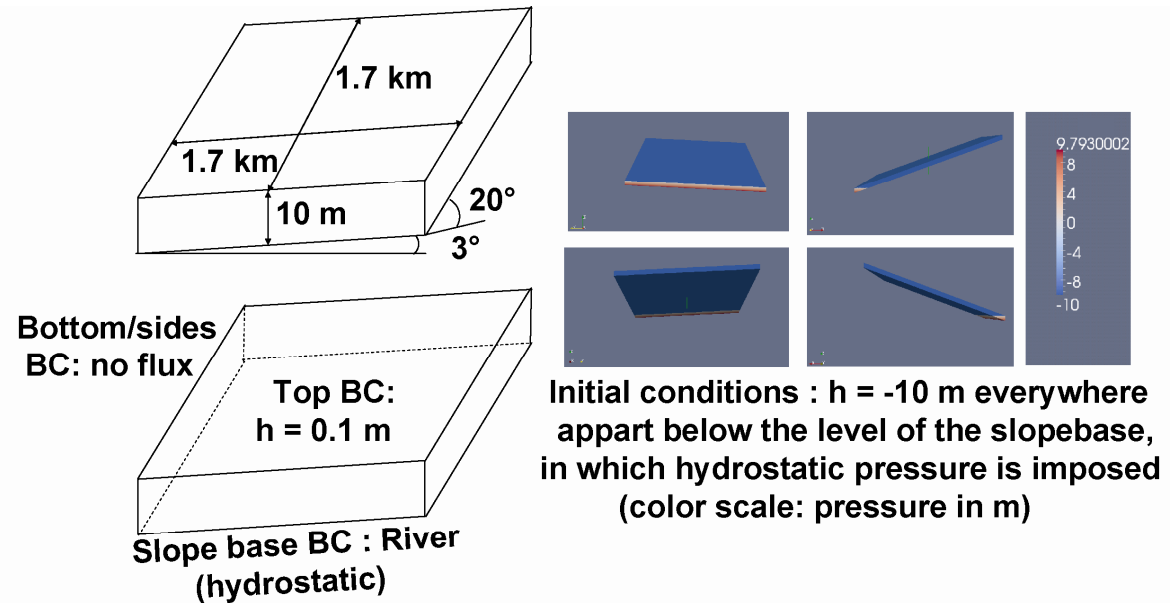
Scaling curves realized on the **CALMIP cluster**

(2944 nehalem cores, DDR infinity Band, Hypercube topology, LUSTRE file system ; www.calmip.cict.fr)

Strong scaling: study of the parallel acceleration

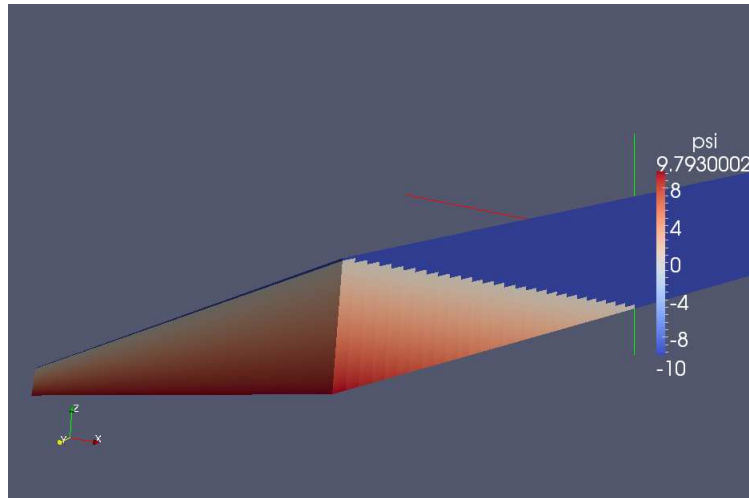
3D subsurface flow in a sloping soil

- slope of 2,9 km² and 10 m of thickness, loamy soil.
- Infiltration on a dry slope
- Ten days of infiltration
- Convergence study: a mesh of 2m*2m*0,2 m cells (~36 millions)

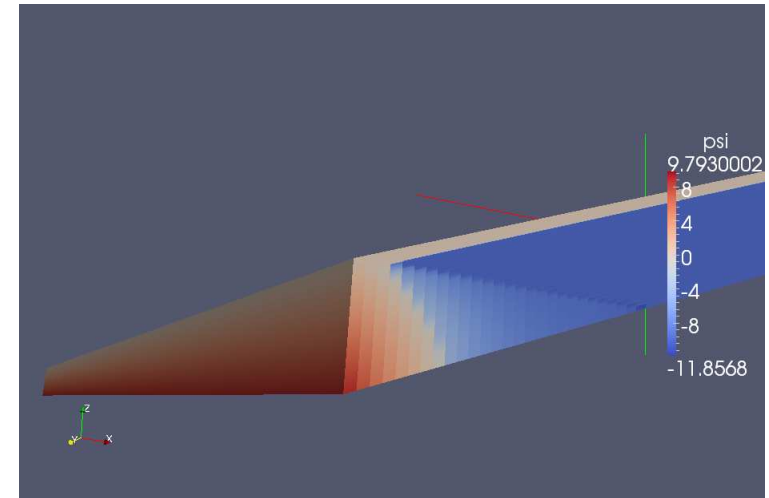


Strong scaling : same problem, more and more processors

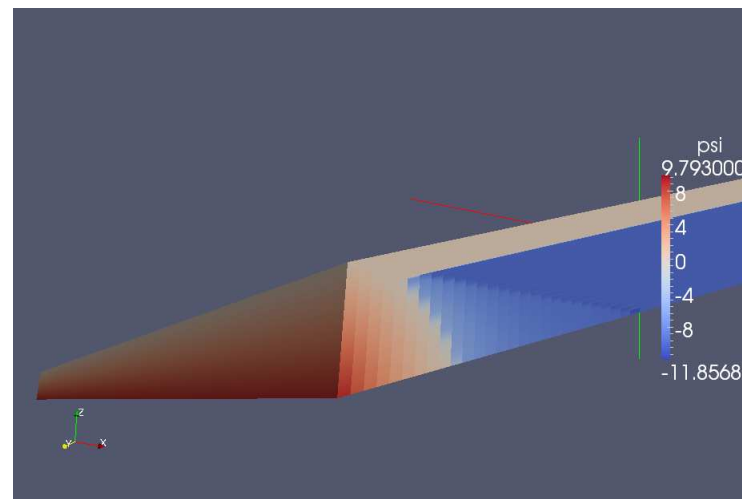
Strong scaling: study of the parallel acceleration



initial



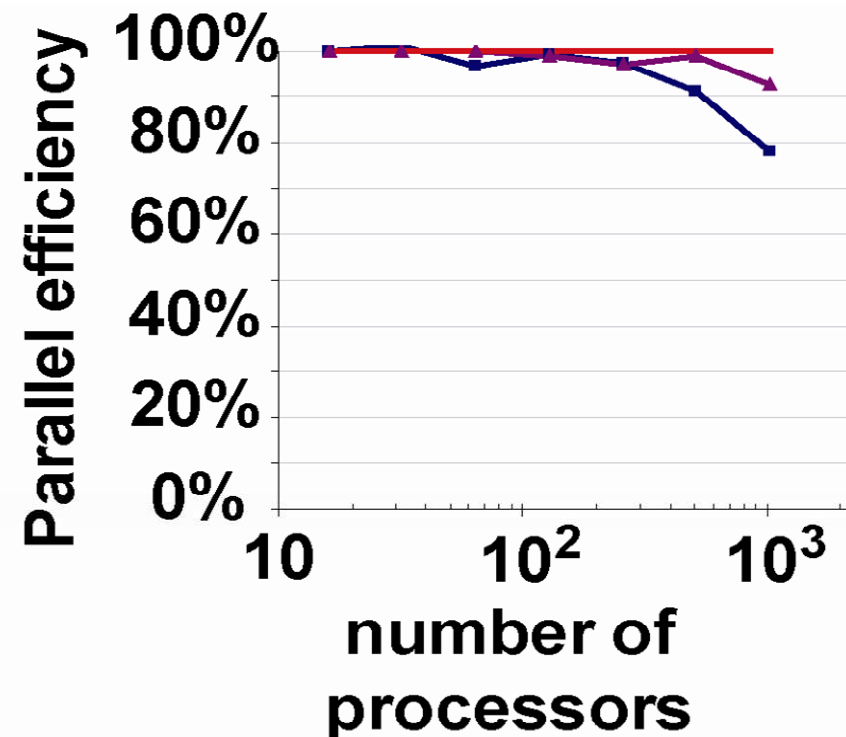
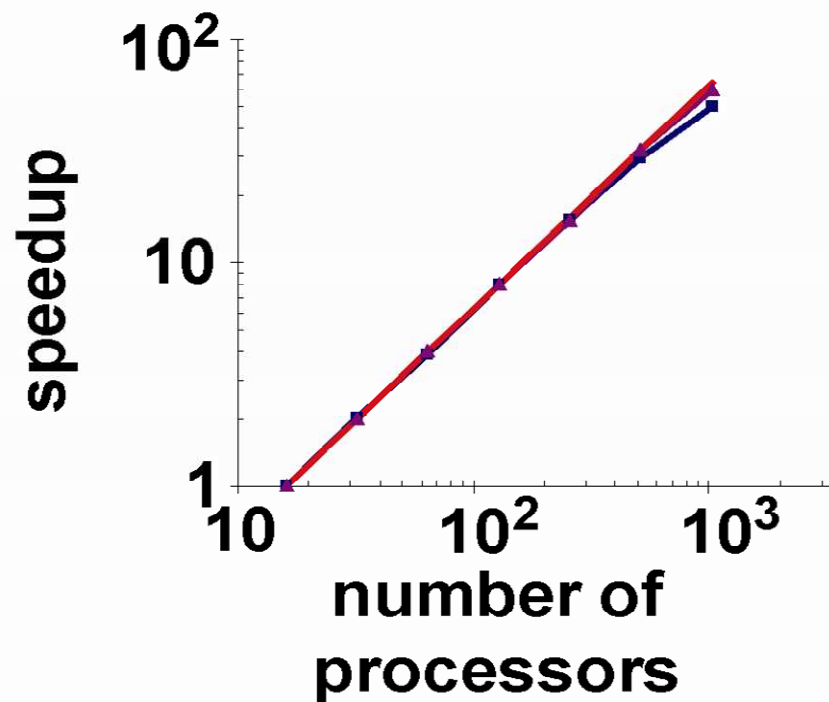
t = 5 j



t = 10 j

Strong scaling: study of the parallel acceleration

— With I/O — Without I/O — Ideal case

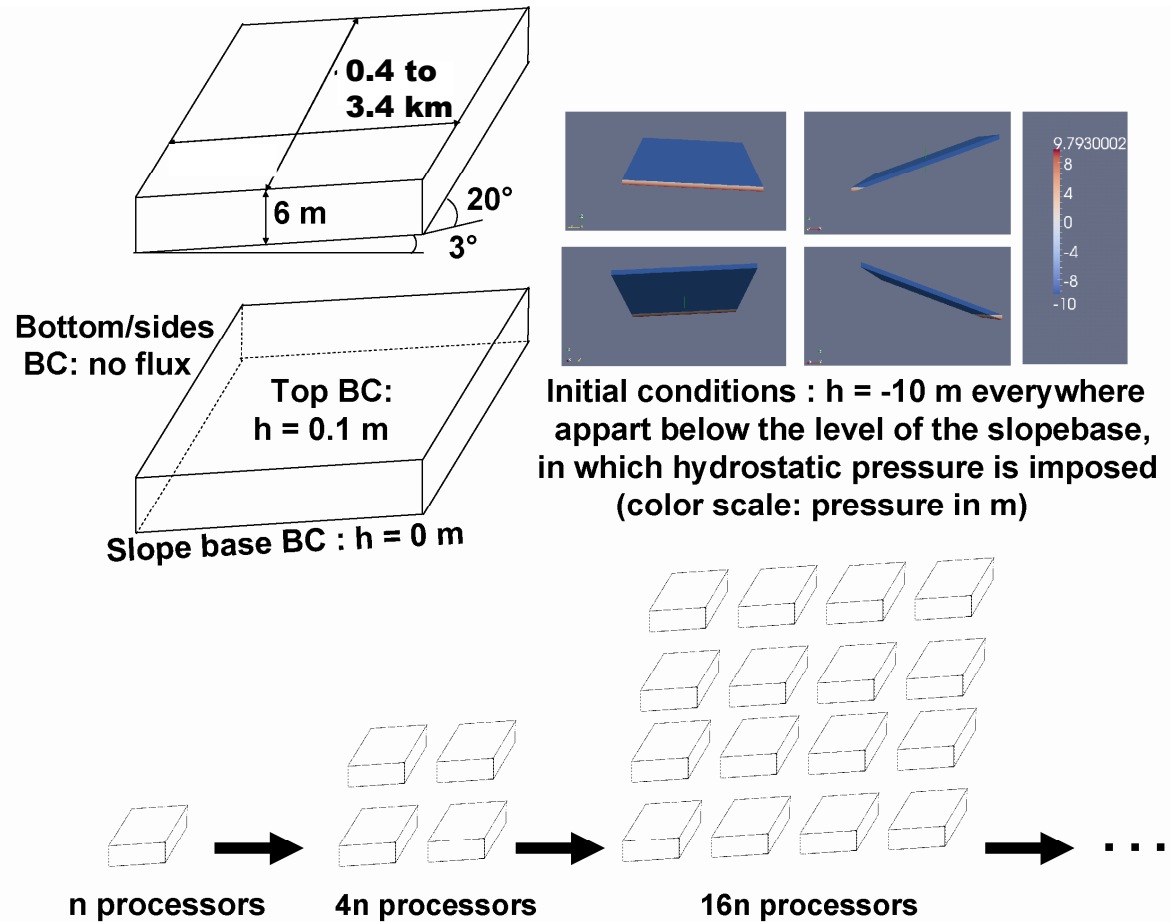


Computation times between ~1h30 (16 cores) and ~2 mn (1024 cores).

(performed on the CALMIP cluster, www.calmip.cict.fr)

Weak scaling: study of the sizing behaviour

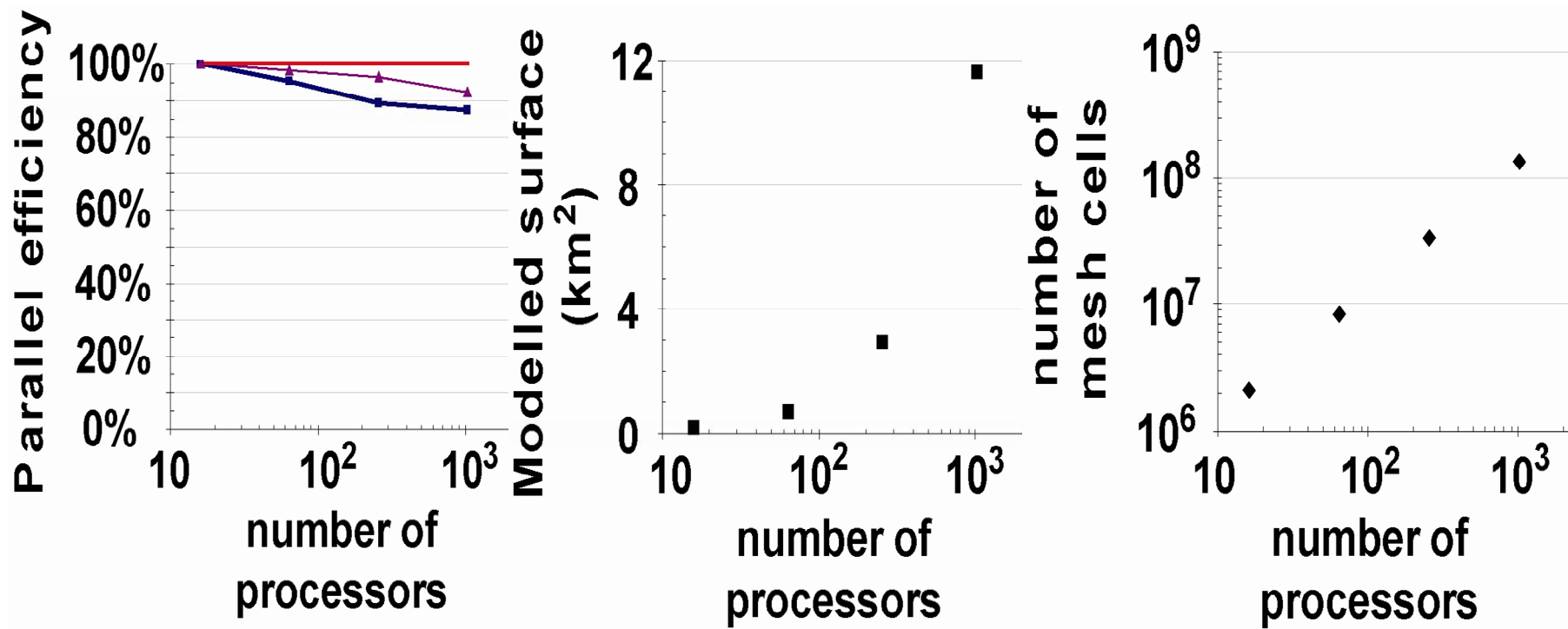
- slopes of 0,2 to 11,6 km² and 6 m of thickness
- ~2 to ~134 millions of cells
- dry slope at the initial time and infiltration occurs
- ten days of infiltration
- parallel meshing and conditioning.



Weak scaling : bigger and bigger problems as well as more and more processors

Weak scaling: study of the sizing behaviour

— With I/O — Without I/O — Ideal case

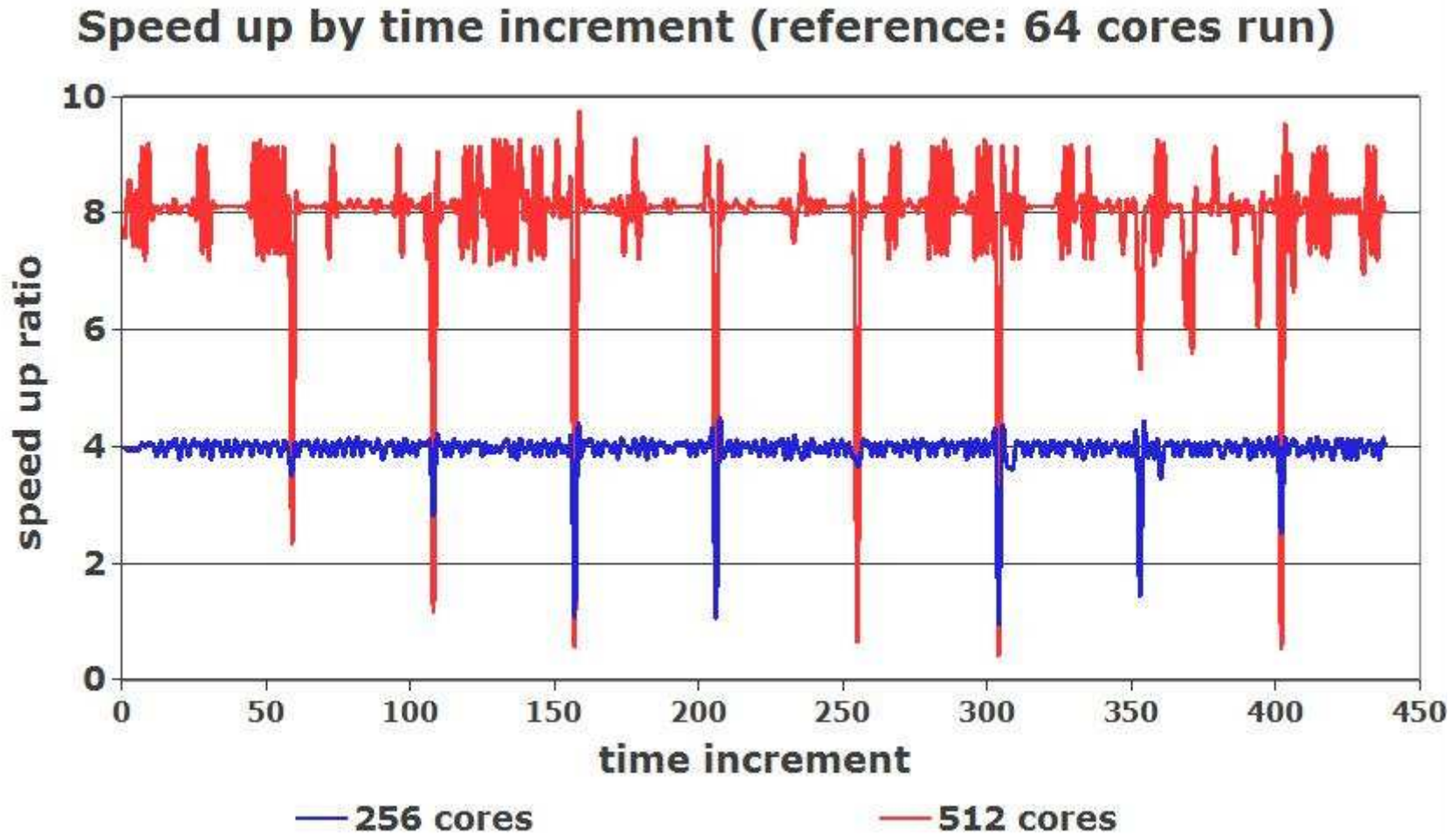


Computation times ~5 mn

(performed on the CALMIP cluster, www.calmip.cict.fr)

Impact of the I/O !

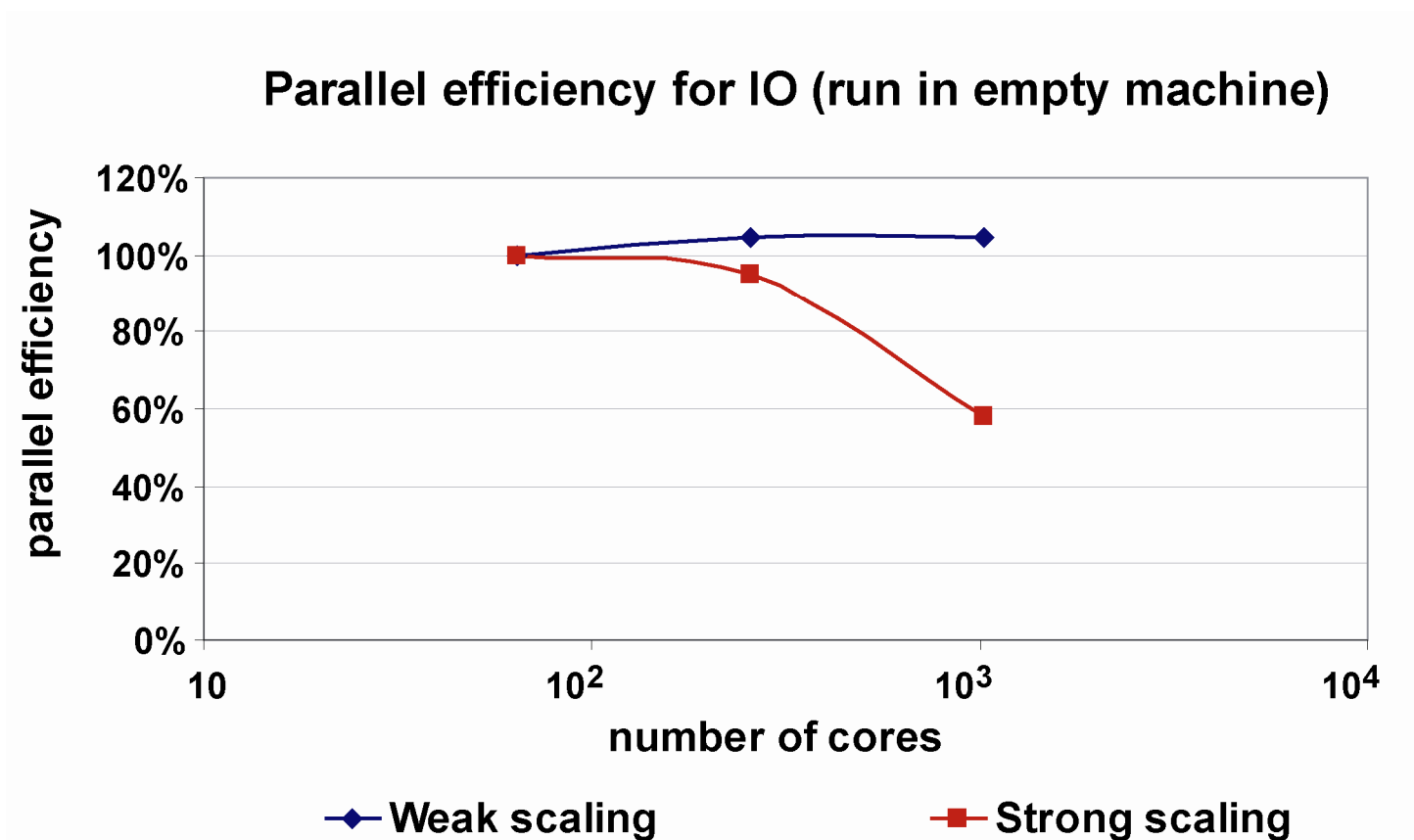
Example of iteration level analysis of strong scaling computations



(performed on the CALMIP cluster, www.calmip.cict.fr)

Study on empty machine to isolate I/O effects

A power outage at the campus allow us to rerun some jobs in an empty machine, thus eliminating the « production effect » on I/O.



(performed on the CALMIP cluster, www.calmip.cict.fr)

Conclusions and perspectives

Conclusions:

RichardsFOAM exhibits **good parallel performances**, both for acceleration (strong scaling) and treatment of large scale cases (weak scaling).

The time scale of the **century** and the space scale of the tens of **square kilometers** is reachable on available supercomputers.

Perspectives:

Coupling with energy and solute transfers

Create meshes from DEMs and geological models

Application to experimental watersheds

(e.g.: ORE-BVET, GDRI CAR WET SIB, MSEC)



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Thank you for your attention

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