RichardsFOAM: high performance computing for the resolution of Richards equation

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Transfers of water in soils

- agriculture (nitrates transfer, …)
- environmental engineering (waste storage, …)
- earth sciences (weathering processes, …)
Flow in unsaturated porous media: Richards equation

Flow in water saturated soils:

\[ S(x) \frac{\partial h}{\partial t} = \nabla \cdot (K(x) \nabla (h + z)) \]

- \( S \) the storage coefficient \([L^{-1}]\)
- \( K \) the permeability tensor \([LT^{-1}]\)
- \( z \) the vertical coordinate \([L]\)
- \( h \) the matrix potential \([L] \left( = \frac{p}{\rho_{\text{water}} g}, h \geq 0 \right)\)

Flow in unsaturated soils: basically two-phase (air-water) flow, and thus two equations of conservation, but ...
Flow in non-saturated porous media: Richards equation

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

\[
c(h, x) \frac{\partial h}{\partial t} = \nabla \cdot (k(h, x) K(x) \nabla (h + z))
\]

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

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

\(c(h)\) and \(k(h)\) functions: experimentally fitted following various models (e.g. van Genuchten 1980, Brooks and Corey 1964)
Flow in non-saturated porous media: Richards equation

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

\[ c(h, x) \frac{\partial h}{\partial t} = \nabla \cdot (k(h, x) K(x) \nabla (h + z)) \]

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

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

Non linearities
Mechanistic modelling at large scales?

(i) Mechanistic modelling (here, numerical solution 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, Goddéris et al., 2012).

(iii) These large scales imply huge memory needs and long computation times.

(iv) Usual approach 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, Šimůnek 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® (Orgogozo et al., CPC 2014)

RichardsFOAM Validation ? Parallel performances ?
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 massive 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 : Preconditionned Conjugate Gradient (Diagonal Incomplete Cholesky preconditionner)
Validations: analytical and code-to-code

Analytical validation

1D stationary cases of evaporation/infiltration with exponential soil properties
(adapted from Tracy 2006)

Comparison with Hydrus 1D (PC Progress)

1D transient infiltration case
(e.g.: Šimůnek et al., 1998, 2008)

Good agreements
Example of application of RichardsFOAM: India

**groovyBC:** building of the top BC on the basis of the hydrologic data chronicles.

Illustrative example: heterogeneous soil column (3 layers) monitored in Karnataka state.

Turmeric field.

Monsoon climate.
Example of application of RichardsFOAM: India

Estimated top BC:
Time dependent Neumann BC

Manual fitting of the soil hydrodynamic parameters
Mean error: 8%
Obs. uncertainties: ~20%
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** Hyperion, in production until 2014

(2944 nehalem cores, DDR infiny Band, Hypercube topology, LUSTRE file system 3 Go/s ; 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)

Initial conditions: h = -10 m everywhere apart below the level of the slopebase, in which hydrostatic pressure is imposed (color scale: pressure in m)

Strong scaling: same problem, more and more processors
Strong scaling: study of the parallel acceleration

initial

$\text{t = 5 j}$

$t = 10 \text{ j}$
Strong scaling: study of the parallel acceleration

Computation times between ~1h30 (1 node, 16 cores, ~2M cells/core) and ~2 mn (128 nodes, 1024 cores, ~0.033M cells/core).

(performed on the CALMIP cluster Hyperion, 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 (snappyHexMesh)

- parallel conditioning (funkySetFields).

Weak scaling: bigger and bigger problems as well as more and more processors.
Weak scaling: study of the sizing behaviour

Computation times ~5 mn (from 1 to 128 nodes, 16 to 1024 cores, ~0.13M cells/core)

(performing on the CALMIP cluster Hyperion, www.calmip.cict.fr)
Impact of the I/O!

(perform on the CALMIP cluster Hyperion, www.calmip.cict.fr)
A power outage at the campus allow us to rerun some jobs in an empty machine, thus eliminating the « production effect » on I/O.

(performing on the CALMIP cluster Hyperion, www.calmip.cict.fr)
Dealing with a large mesh: 1.2 billion cells strong scaling

- With a development version of OpenFOAM (https://github.com/OpenFOAM/OpenFOAM-dev)
- Same kind of 3D subsurface flow that for the strong scaling study: slope of 11.6 km², 20m thickness, loamy soil. Infiltration on a dry slope for 10 days.
- Number of mesh cells: ~1.2 billion (1m*1m*0.2m cells)
- CALMIP cluster: Supercomputer EOS*, 12240 cores, IVYBRIDGE 2.8Ghz processors, Infiniband FDR, fat tree non-blocking topology, LUSTRE file system 10 Go/s, in production since 2015)
- Investigated number of cores: from 400 to 1600
- Time of mesh building: 8 hours on UVPROD* (1.5 TB RAM request)
- Time of mesh decomposition: from 21 hours to 67 hours on UVPROD* (from 0.75 TB RAM to 1.5 TB RAM requests)

* See www.calmip.univ-toulouse.fr for more details.
Dealing with a large mesh: 1.2 billion cells strong scaling

Computation times between ~5h10 (400 cores, ~3M cells/core) and ~37mn (3200 cores, 0.375M cells/core).

(Performed on the CALMIP cluster EOS, www.calmip.cict.fr)
Dealing with a large mesh: 1.2 billion cells strong scaling

Computation times between ~5h10 (400 cores, ~3M cells/core) and ~37mn (3200 cores, 0.375M cells/core).

(Performed on the CALMIP cluster EOS, www.calmip.cict.fr)
Impact of the heterogeneity of the medium: no spatial correlations

- 3 porous media of 20m*10m*10m
- Lognormal distributions of $K_{sat}$
- Increasing standard deviation $\sigma$
- 40 days of Infiltration
- Meshes: 34 millions cells

$K_{sat}$ mean: $10^{-6}$ m.s$^{-1}$; $K_{sat}$ maximum range: $10^{-3} – 10^{-10}$ m.s$^{-1}$
Impact of the heterogeneity of the medium: no spatial correlations

Infiltration of water on 3D blocks (20m*10m*10m) of heterogeneous soil

**Saturated zone**
- BC: Zero flux, IC: psi=5m
- IC: psi=5m

**Unsaturated zone**
- BC: Zero flux, IC: psi=5m
- BC: imposed pressure, psi= -0.1m, IC: psi= -5m

Mean $K_s = 10^{-6}$ m.s$^{-1}$; $\alpha = 3.6$ m$^{-1}$; $n = 1.56$; $\theta_s = 0.43$; $\theta_r = 0.078$

Impact of the heterogeneity of the medium: no spatial correlations

\[
\frac{\sigma(\ln(K_{sat}))}{\text{mean}(\ln(K_{sat}))} = 0.316 : \sim 11\ 500
\]
\[
\frac{\sigma(\ln(K_{sat}))}{\text{mean}(\ln(K_{sat}))} = 1 : \sim 12\ 500
\]
\[
\frac{\sigma(\ln(K_{sat}))}{\text{mean}(\ln(K_{sat}))} = 3.16 : \sim 33\ 000
\]

(performed on the CALMIP cluster Hyperion, www.calmip.cict.fr)
Spatially correlated media: preliminary tests

Increasing correlation length (m)

5 porous media of 10m*10m*10m (8 millions mesh cells)

1 spatially uncorrelated medium

3 spatially correlated media with increasing spatial correlation lengths (0.2m, 1m, 5m) – turning band generation method

1 spatially constant medium

lognormal distributions (+1 cst),
mean\( (K_{sat}) = 10^{-6} \) m.s\(^{-1}\),
\( \sigma(\ln(K_{sat})) / \text{mean}(\ln(K_{sat})) \sim 1 \)

0.5 days of Infiltration
Spatially correlated media: preliminary tests

Infiltration of water on 3D blocks (10m*10m*10m) of heterogeneous soil

BC: imposed pressure, psi = 1m, IC: psi = -5m

BC: Zero flux, IC: hydrostatic

BC: Zero flux, IC: psi = 5m

BC: hydrostatic

BC: Zero flux, IC: hydrostatic

Mean $K_s = 10^{-6} \text{ m.s}^{-1}$; $\alpha = 3.6 \text{ m}^{-1}$; $n = 1.56$; $\theta_s = 0.43$; $\theta_r = 0.078$
Spatially correlated media: preliminary tests

(performed on the CALMIP cluster EOS, www.calmip.cict.fr)
Spatially correlated media: preliminary tests

Execution time with 500 cores

Parallel efficiency at 500 cores

Total number of PCG iterations with 500 cores
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
App. to experimental watersheds in India, Russia, Lao PDR (e.g.: ORE-BVET, GDRI CAR WET SIB, MSEC)
RichardsFOAM_2

- Direct handling of fully heterogeneous porous media ($K_{sat}$ as well as $\alpha$, $n$, $\theta_s$, $\theta_r$)

- Computation of water fluxes at faces for fixed flux BC and for transport modelling

- Direct computation of actual evapotranspiration on the basis of potential evapotranspiration
Thank you for your attention.

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