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An open source massively parallel solver for Richards equation: Mechanistic modelling of water fluxes at the watershed scale☆

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ABSTRACT

In this paper we present a massively parallel open source solver for Richards equation, named the RichardsFOAM solver. This solver has been developed in the framework of the open source generalist computational fluid dynamics tool box OpenFOAM® and is capable to deal with large scale problems in both space and time. The source code for RichardsFOAM may be downloaded from the CPC program library website.

It exhibits good parallel performances (up to ∼90% parallel efficiency with 1024 processors both in strong and weak scaling), and the conditions required for obtaining such performances are analysed and discussed. These performances enable the mechanistic modelling of water fluxes at the scale of experimental watersheds (up to few square kilometres of surface area), and on time scales of decades to a century. Such a solver can be useful in various applications, such as environmental engineering for long term transport of pollutants in soils, water engineering for assessing the impact of land settlement on water resources, or in the study of weathering processes on the watersheds.

Program summary

Program title: RichardsFOAM

Catalogue identifier: AEUF_v1_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEUF_v1_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: Standard CPC licence, http://cpc.cs.qub.ac.uk/licence/licence.html

No. of lines in distributed program, including test data, etc.: 1287

No. of bytes in distributed program, including test data, etc.: 9521

Distribution format: tar.gz

Programming language: C++.

Computer: any x86, tested only on 64-bit machines.

Operating system: Generic Linux.

Classification: 13.

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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External routines: OpenFOAM® (version 2.0.1 or later)

Nature of problem:
This software solves the non-linear three-dimensional transient Richards equation, which is a very popular model for water transfer in variably saturated porous media (e.g.: soils). It is designed to take advantage of the massively parallel computing performance of OpenFOAM®. The goal is to be able to model natural hydrosystems on large temporal and spatial scales.

Solution method:
A mixed implicit (FVM in the object oriented OpenFOAM® framework) and explicit (FVC in the object oriented OpenFOAM® framework) discretization of the equation with a backward time scheme is coupled with a linearization method (Picard algorithm). Due to the linearization loop the final solution of each time step tends towards a fully implicit solution. The implementation has been carried out with a concern for robustness and parallel efficiency.

Restrictions:
The choice of the maximum and initial time steps must be made carefully in order to avoid stability problems. A careful convergence study of mesh cell size, linear solver precision and linearization method precision must be undertaken for each considered problem, depending on the precision required for the expected results, the spatial and temporal scales at stake, and so on. Finally, the solver in its current version only handles meshes with a constant cell volume (a crash will not necessarily occur with an irregular mesh but some problems may arise with the convergence criterion of the linearization method).

Running time:
Highly variable, depending on the mesh size and the number and nature of cores involved. The test run provided requires less than 2 s on a 64 bit machine with Intel® CoreTMi7-2760QM CPU @ 2.40 GHz × 8 and 3.8 Gigabytes of RAM.

1. Introduction

Many applications in the geosciences involve transfers of water in variably saturated porous media, such as soils. From the point of view of water engineering, the direct infiltration of rainwater into soils is the main recharge of aquifers, and is also their main source of pollution, for instance through infiltration of dissolved nitrates and pesticides. Accurate modelling of water transfer in soils is thus important for water engineering applications. On the other hand, water transfer in porous media controls water content in the soil profile, which is one of the driving parameters of weathering [1], the key process in the carbon cycle [2].

It is generally admitted (for example, [3–5]) that mechanistic approaches are the "gold standard" [5] for modelling natural water systems, since they allow quantitative and predictive assessment of water flows. Such tools are thus of great interest for studying the impact of global changes on weathering processes, which requires modelling under evolving climatic conditions (e.g.: "dry" or "wet" warming). The design of water management infrastructures (e.g.: dams, wells) also leads to the necessity of modelling the water transfers within changing water systems, and thus requires the use of mechanistic modelling approaches. In order to perform mechanistic modelling of water flows in soils, it is necessary to be able to quantitatively assess the spatial and temporal evolution of water pressure and water content. The most widely used approach in order to reach this goal is numerical resolution of the three dimensional Richards equation [6]. This equation is an approximate solution of the general two-phase flow in porous media model based on generalized Darcy's laws [7], assuming that the pressure gradient in the gas phase is small. This assumption may be questionable under certain circumstances, in particular trapped gas phase in less permeable lenses. Similarly, the generalized Darcy's law model itself is not entirely supported by upscaling theories ([8–13]; etc.) and is the subject of current research. However, up to now, Richards equation is still the model of choice in engineering practice and provides applicable results in many cases. In addition, Richards equation is used in applications other than the modelling of natural water system, such as nuclear waste repository (e.g.: [14]) or proton exchange membrane fuel cell (e.g.: [15]).

Richards equation is based on Darcy's law with pressure-dependent, or moisture dependent, hydraulic conductivity. It is applicable under the usual conditions of pressure and temperature, with water considered an incompressible fluid, with the air phase remaining connected to the atmosphere (fixed air pressure) and having a negligible viscosity. Additionally, the hysteresis effects that may be encountered in the case of successive imbibition/drainage cycles [16] are neglected in this work. The Richards approach then leads to the following governing equation for water flow in a variably saturated porous medium:

$$\frac{\partial \theta}{\partial t} = C\,(h)\,\frac{\partial h}{\partial t} = \nabla .\,(\mathrm{K}\,(h)\,.\nabla\,(h+z))\,. \tag{1}$$

In this equation, h is the pressure head expressed as length of water column (m), z is the vertical coordinate (m) (oriented upward), $K(h)$ is the hydraulic conductivity of the unsaturated porous medium (m s^{-1}), $\theta(h)$ is the volumetric water content (m^3 m^{-3}) and $C(h)$ is the capillary capacity (also called specific moisture capacity) of the unsaturated porous medium (m^{-1}). Leaving $\partial\theta/\partial t$ on the left hand side leads to the so-called mixed formulation of the Richards equation in numerical implementations. With $C(h)\partial h/\partial t$ on the left hand side, we have the pressure formulation of Richards equation, which is that adopted in this work, and is also historically the original equation of Richards [6]. Water content formulations also exist, but they are limited to strictly unsaturated situations without the possibility of pressure build up in saturated zones. One can refer to [17] for a detailed discussion of the mixed formulation for implicit 3D finite volumes, and to [18] for a systematic comparison of these various formulations for 1D unsaturated flows.

The main complexity of the Richards equation lies in the non-linearities due to the pressure dependent hydraulic conductivity $K(h)$ and of the pressure dependent capillary capacity $C(h)$. These dependencies, as well as the water content–pressure relationship (the water retention curve $\theta(h)$), are treated with empirical models such as that of Brooks and Corey [19] or the van Genuchten