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A scalable coupled surface–subsurface flow model

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ABSTRACT

The coupling of physically-based models for surface and subsurface water flows is a recent concern. The study of their interactions is important both for water resource management and environmental studies. However, despite constant innovation, physically-based simulations of water flows are still time consuming. That is especially problematic for large and/or long-term studies, or to test a large range of parametrizations with an adjoint model. As the current trend in computing sciences is to increase the computational power with additional computational units, new model developments are expected to scale efficiently on parallel infrastructures. This paper describes a coupled surface–subsurface flow model that combines implicit and explicit time discretizations for the surface and subsurface dynamics, respectively. Despite that the surface flow has a faster dynamics than the subsurface flow, we are able to use a unique nearly-optimal time step for each submodel, hence improving the resources use. The surface model is discretized with an implicit control volume finite element method while the subsurface model is solved by means of an explicit discontinuous Galerkin finite element method. The surface and subsurface models are coupled by weakly imposing the continuity of water pressure. By imposing a threshold on the influence coefficients of the control volume finite element method, we can prevent the occurrence of unphysical fluxes in anisotropic elements. The proposed coupling is shown to produce results similar to state-of-the-art models for four different test cases while achieving better strong and weak scalings on up to 192 processors.

1. Introduction

The anthropogenic impact on the environment intensifies continuously with the expansion of the population and the development of its standard of living. To study how human activities influence its surrounding environment, it is important to fully understand the biogeochemical exchanges across the biosphere. Such exchanges are mainly driven by surface and subsurface water flows, which are difficult to predict without appropriate tools. Numerical models are increasingly used for this purpose.

Physically-based models are competing with statistically-based models. The formers are based on complex mathematical equations that can be difficult to parametrize [1] but with the added value of an understanding of the underlying processes. The laters, based on simple generic formulas, can provide an easy and precise fit with observations data but lack of flexibility when a change occurs in the system [2]. It is possible to mix both approaches with an uncertainty analysis to assess the variability of the results [3]. The main sources of uncertainty of physically-based models are the physical model hypotheses, the mathematical approximations, the numerical discretization, the heterogeneity and variability of the parameters, and the calibration of non-linear models with uncertain measures.

In a physically-based model of the terrestrial water cycle, the processes are usually modeled by means of the shallow water equations for the surface flows and the Richards' equation for the subsurface flows. The shallow water equations are a convenient 2D approximation of the full 3D Navier–Stokes equations when the water height is small, which is the case for surface flows. It can be complemented by additional 1D equations for rivers and channels to handle the jump in the physical process scales. The Richards' equation approximates the soil as a porous medium with highly non-linear parameters. It assumes an isothermal and laminar flow with no chemical gradients or inertial forces and water as the unique fluid phase, hence neglecting the air component [1]. It can be complexified by adding hysteresis, fractures, multiple phases or macropores, although those extensions are difficult to

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spatialize and parametrize. Since the physical complexity of the shallow water equations goes beyond what is required for surface–subsurface flow interactions, simpler models are generally used. The most popular ones are the non-inertia or diffusive wave model and the kinetic wave model. Some simplified approaches based on the kinetic wave equation are going further in the approximations, simulating the surface water via a tree-structured network of water reservoirs, following the topographical slopes [4]. While being fast, this method is based on strong underlying hypothesis and is hence inappropriate for natural reservoirs. Among the many existing approaches [5–7], a state-of-the art method to discretize the non-inertia equation is the control volume finite element (CVFE) method, also called the influence coefficient method [8–12]. This method applies upwind fluxes between the nodes of a mesh element. Its main advantage over the classical continuous Galerkin formulation is to avoid the issues related to zero or negative water depths. As the non-inertia equation is nearly elliptic when the water height becomes significant, an implicit time integration scheme is recommended.

The numerical discretization of the Richards' equation has been extensively studied, as it presents various numerical difficulties such as unphysical oscillations, mass conservation errors or a lack of robustness. These issues can be partly circumvented by carefully selecting the non-linear solver [13,14] as well as the space discretization [9,15,16]. Most Richards' equation models rely on implicit time integration schemes and hence present convergence issues [17] or sub-optimal scaling on parallel infrastructures [18–23]. The time step of implicit time integration schemes is unrestricted for simple diffusion equations, but the non-linearities of the Richards' equation put an upper limit to it [17]. Recently, De Maet et al. [24] have proposed a model using an explicit time integration scheme and a discontinuous Galerkin (DG) finite element (FE) spatial discretization. Such an approach achieves an optimal strong scaling as it does not require linear or non-linear solvers and hence avoids the associated convergence issues. It relies on the use of slope limiters to increase the scheme robustness and a special DG interface term that allows physical discontinuities in the water content at the elements interface. The interface between two different soils is precisely represented by the DG FE approximation, therefore no mixing between the different properties is necessary as it is the case in continuous Galerkin FE models. A detailed review of Richards' equation models can be found in [16].

In the last decade, the coupling of the shallow water equations and the Richards' equation has been an increasingly active domain of research (see for instance [25] or [26] for an overview). The complexity of studies in this field are mostly due to the fact that surface and subsurface interactions are difficult to measure. Another issue is the difficulty to model water fluxes that often exhibit a large spatial and temporal variability. Indeed, processes occurring at small spatial scales, like river flows, coexist with processes occurring at large spatial scales, like groundwater flows. Similarly, slow processes like the dynamics of the vadose zone coexist with rapid processes like surface runoff.

In a continuous world, when surface water is present, the most physically consistent coupling is to match the hydrostatic pressure of the surface flow with the pressure head of the subsurface flow at the top of the soil layer [18,12]. However, a pressure continuity (PC) coupling strategy would require the soil to be discretized up to the scale of the smallest water fluxes between surface and subsurface, which is rarely feasible in practice because of the associated computational cost. Additionally, the small features of the surface linked to those specific fluxes, such as the microtopography, the surface soil compression and vegetation cover, are often very difficult to estimate. Eventually, such a coupling strategy requires the surface and subsurface models to be connected in one non-linear solver step. The solution is then provided either by iterative coupling methods, which require multiple iterations per time step, or by an implicit time integration scheme, which produces a non-linear system that is often difficult to solve and scales poorly on parallel architectures. Another coupling is the first-order exchange coefficient (FOEC) coupling for which the pressure continuity is weakly imposed [9,10,12]. The FOEC coupling allows the surface and subsurface to be solved separately and it can assume additional sub-scale physics at interfaces. It converges towards the PC coupling when the coefficient tends towards infinity. With an appropriate choice of coefficient it can produce results very close to the PC coupling with enhanced model performances [27,28].

Although the research on coupled surface–subsurface models is well developed, none of the current models achieve an optimal scaling on parallel architectures. For Richards' equation, the parallel efficiency (defined as the fraction of available computational resources fully-used) of a model like PARSWMS is of 75% but it can decrease to 29% in some cases [20]. For the coupled model PARFLOW, the efficiency varies between 40% and 72% [18]. As a general rule of the thumb, performances decrease with the number of computational units and increase with the number of degrees of freedom allocated to each computational unit. This is mainly due to the complexity of the global system solution, which requires many communications to exchange information between subdomains. That amount of communications limits the parallel efficiency, especially when a large number of nodes is involved. Those performances are likely to keep decreasing in the future with the use of newer technologies. Indeed, today new computers increase their power by adding more computational units. That implies a change of paradigm for computational code development as individual computing units are no longer increasing in power. Instead, the number of computing units increases. To use all capabilities of future devices, adapted algorithms have therefore to be developed to achieve efficient parallel codes.

In this paper, we present a coupled surface–subsurface flow model that combines an implicit model for the non-inertia shallow water equation and an explicit model for the Richards' equation [24]. Such an approach allows us to use the same time step for both models, as the slow dynamics of the groundwater requires an explicit time step close to the implicit time step required for convergence of the surface flow non-linear solver. Despite using an implicit scheme for the surface model, the overall scaling is still nearly optimal as the subsurface model generally needs the largest part of the computational resources. The FE method has been selected mostly for its ability to solve the model equations on unstructured meshes, which are well suited to complex geometries such as real catchments. Its CVFE declination for surface flow is close to a finite volume method, increasing first the robustness and then the scheme convergence. Its DG FE declination for subsurface flow allows for physical discontinuities of the water content and for the use of limiters to also increase the scheme robustness. As both the non-inertia and the Richards equations are strongly non-linear, robustness is often favored over precision, which would be achieved for instance by a higher order spatial discretization. The use of similar spatial discretizations for the surface and the subsurface models allows an easier coupling, as each surface element has a unique corresponding subsurface element face. We introduce a flexible coupling approach that lies between an exact surface–subsurface pressure coupling, and the FOEC formulation. This hybrid coupling comes together with the DG FE method when using its Dirichlet boundary condition. It has the advantages to be easier to solve than a direct coupling, as it is less stringent, to converge towards the pressure continuity coupling after a transitory