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A GPGPU-accelerated implementation of groundwater flow model in unconfined aquifers for heterogeneous and anisotropic media

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ABSTRACT

The application of computer simulation models plays a significant role in the understanding of water dynamics in basins. The recent and explosive growth of the processing capabilities of General-Purpose Graphics Processing Units (GPGPUs) has resulted in widespread interest in parallel computing from the modelling community. In this paper, we present a GPGPU implementation of finite-differences solution of the equations of the 2D groundwater flow in unconfined aquifers for heterogeneous and anisotropic media. We show that the GPGPU-accelerated solution implemented using CUDA[1] C/C++ largely outperforms the corresponding serial solution in C/C++. The results show that the GPGPU-accelerated implementation is capable of providing up to a 56-fold speedup in the solution using an ordinary office computer equipped with an inexpensive GPU[2] card. The code developed for this research is available for download and use at http://modelagemambientaluffs.blogspot.com.br/.

1. Introduction

Spatially distributed models are widely recognized as important tools for the understanding of groundwater dynamics (Markstrom et al., 2008; Rouholahnejad et al., 2012; Zhang et al., 2013; Hwang et al., 2014; Le Phong et al., 2015). They are widely applicable in environmental analysis of flooded areas, pollutant contamination of aquifers, wells and reservoirs (Botros et al., 2012; Czarnecki et al., 2010; Allan Freeze and Witherspoon, 1966; He et al., 2011; Hwang et al., 2014; Lamb and Beven, 1997; Lange et al., 2014; Le Phong et al., 2015; Lyne and Hollick, 1979; Miller et al., 2013; Markstrom et al., 2008; Mendoza and Martins, 2006; Voeckler et al., 2014). The implementation of computer models has benefited from the rapid growth in computational capabilities observed over the last thirty years or so (Lange et al., 2014; Markstrom et al., 2008). More recently, the rapid emergence of parallel computing platforms based on GPGPU (General Purpose Graphics Processing Units) has provided an entirely new perspective regarding the processing capabilities of personal computers, thus attracting the attention of the modelling community (Nickolls et al., 2008; Singh et al., 2011; Ji et al., 2012, 2014; Le Phong et al., 2015; Zhou et al., 2013). In this context, hydrological models are particularly suitable for massively parallel frameworks due to the state-of-the-art of solution techniques for sparse linear systems via domain decomposition methods (Barrett et al., 1994; Formaggia et al., 2006).

The assessment of groundwater and surface water dynamics in real basins is a challenging issue which requires knowledge of several factors that influence the hydrological cycle, such as the physical and chemical characteristics of the soil and of the environment as a whole. A number of studies have been devoted to the development of hydrologic models whose aim is to describe groundwater flow while considering different levels of soil saturation and diverse geologic conditions (Freeze, 1971; Lange et al., 2014; Voeckler et al., 2014). Among the variety of groundwater models in the literature, one can find models that describe groundwater flow in basins (Graaf et al., 2014; Czarnecki et al., 2010; Freeze, 1971; Marc et al., 1998). Most commonly, groundwater models are designed to deal with the case of isotropic and homogeneous media (Harbaugh, 2005; Markstrom et al., 2008; Lange et al., 2014; Voeckler et al., 2014; Czarnecki et al., 2010). Although the assumptions on homogeneity and isotropy permit the simplification of the resulting equations and their solution, they might not be adequate in describing more general situations in which the flow media is recognized to be substantially heterogeneous (Heath, 1983; Wainwright and Mulligan, 2004; Harbaugh, 2005).

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[1] Compute Unified Device Architecture.
[2] Graphics Processing Unit.

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Availability

Program name ParGW
Developer Tomas Carlotto
Contact address thomas.carl@hotmail.com
Year first available 2017
Software required CUDA™ Toolkit 8.0 or later and CUSP library
Program language CUDA™ C++
Package size 179 Mb
Availability http://modelagemambientaluffs.blogspot.com.br/
Cost free of charge

Regarding the application of high-performance computing to simulations of water and environment-related phenomena, several publications have shown the advantages of parallel computing frameworks (Le Phong et al., 2015; Ji et al., 2012, 2014; Zhou et al., 2013; Hwang et al., 2014; Nakajima, 2013; Rouholahnejad et al., 2012; Wu et al., 2013; Zhang et al., 2013). The increased efficiency and reduced computational time of parallel frameworks allow for the simulation of physically-based models over large areas with finer grid resolutions (Le Phong et al., 2015; Nakajima, 2013; Ji et al., 2012, 2014). In addition, the reduced computing time enables rapid modelling and analysis during emergency situations in the wake of environmental disasters (Rouholahnejad et al., 2012). In this regard, high-performance computer models can play a fundamental role in reducing the response time following environmental disasters, thus broadening the perspectives of achieving effective engineering solutions for emerging problems.

Recent publications have shown that parallelized computer models are a feasible and affordable means of rapidly assessing engineering solutions. As time is a major concern in the calibration of hydrologic models, the parallelization of calibration algorithms in CPUs has provided increased speedup and scalability (Rouholahnejad et al., 2012). In this context, GPU implementations are expected to provide even greater speedups (Rouholahnejad et al., 2012) due to the increasing number of processors and the amount of memory available. Indeed, in Ref. (Ji et al., 2012), CUDA^{TM}-based solvers were applied to transient groundwater flow problems and achieved roughly a 4-fold speedup. Another noticeable fact of parallel implementations is the finer-grained resolutions for computational mesh grids. Take for instance the parallel implementation of GCSFlow (GPU-based Conjunctive Surface Subsurface Flow Model, which permitted the computation of surface and subsurface water flow for a domain with a topographic resolution of $1.2m \times 1.2m$ (Le Phong et al., 2015). Another example of parallelization related to hydrologic models was the implementation of MODFLOW (McDonald and Harbaugh, 2003; Harbaugh, 2005), in which GPU methods were shown to outperform multi-CPU methods (Ji et al., 2014). In this specific case, the parallelized version of MODFLOW was found to provide a 10-fold speedup in relation to the serial one (Ji et al., 2014). This indicates that the application of GPGPU is a promising path to enhancing massive processing of scientific data.

In this paper, we develop a GPGPU-accelerated implementation of the groundwater flow in unconfined aquifers for anisotropic and heterogeneous media. We generalize results previously published in the literature which consider the case of homogeneous and isotropic media and propose a massively parallel implementation that enables the solution of the groundwater flow problem for heterogeneous and anisotropic soils. There are two main difficulties associated with the numerical solution of this model: (i) the resulting equation is nonlinear, as the hydraulic conductivity depends on the hydraulic head, and (ii) due to the fact that the parameters are state-dependent, the matrix of the corresponding linear system has to be redefined at each time step, which is time-consuming. These issues were solved by (i) considering a quasi-linear approach in which the hydraulic conductivity variable parameter is one step behind the hydraulic conductivity, and (ii) developing a dedicated kernel to redefine the matrix at each time step. The model is discretized using the Crank-Nicolson finite-difference scheme (Crank and Nicolson, 1947, 1996) and then solved using a CUDA™ C/C++ implementation based on CUSP library (Bell and Garland, 2013). The main objective of this research is to provide an efficient and sufficiently general parallel implementation of the groundwater flow model. As a means of testing the solution speedup, we consider the groundwater flow problem for different grid resolutions running CUDA™ C/C++ parallel code and then its serial counterpart in C/C++. The results show that the CUDA™ C/C++ parallel implementation achieves up to a 56-fold speedup in relation to the serial one. The outline of the paper is as follows: the materials and methods are presented in section 2; the GPGPU implementation performance results and application to a real basin are found in section 3; the results are discussed in section 4 and put into perspective with similar studies from the literature; final remarks and future perspectives are dealt with in section 5. future perspectives.

2. Materials and methods

In this section, we present the model equations, the discretization process and the solution method for the resulting linear system using CUDA™.

2.1. The equations for groundwater flow in unconfined aquifers

The groundwater flow can be modelled as the transient behavior of the hydraulic heads. With this in mind, Ref (Boussinesq, 1904; Delleur, 2006; Fetter, 2001). were studied in detail on the basis of the continuity equation and Darcy's law. Considering the hydraulic conductivities K_{xx}, K_{yy}, K_{zz}, Darcy's equation and the continuity equation for mass, a 3D model for groundwater flow for the hydraulic head h can be written as

$$\left(\frac{\partial}{\partial x}\left(\rho.K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(\rho.K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(\rho.K_{zz}\frac{\partial h}{\partial z}\right)\right).\triangle V+\rho.Q.\triangle V = S_s.\frac{\partial h}{\partial t}\triangle V \tag{2.1}$$

in which ρ is the fluid density, $\triangle V$ is the variation in volume, Q is associated with a sink/source term and S_s is the storage term, given by

$$S_s = \rho.g.[\alpha + \eta.\beta]$$

where g is gravity; α is the compressibility of the geologic media, η is the soil porosity and β is the water compressibility (Cleary, 1989). In order to make the model tractable, the following assumptions can be adopted.

- *The fluid is incompressible*, which means the fluid density is constant. This is a reasonable assumption since the model is not dealing with coastal zones (where there is a mix of fresh water and salt water within the soil layers) nor groundwater