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Improving water quantity simulation & forecasting to solve the energy-water-food nexus issue by using heterogeneous computing accelerated global optimization method

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HIGHLIGHTS

- We proposed a novel parallel SCE-UA method.
- We implemented the parallel SCE-UA on multi-core CPU and many-core GPU.
- The parallel SCE-UA can obtain global optimum much faster than original serial version.

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ABSTRACT

With continuous population increase and economic growth, challenges on securing sufficient energy, water, and food supplies are amplifying. Water plays the most important role in the energy-water-food (E-W-F) nexus issue such as energy supply (clean hydropower energy generation), water supply (drinking water), and food supply (agricultural irrigation water). Therefore, water quantity simulation & forecasting become an important issue in E-W-F nexus problem. Water quantity simulation & forecasting model, such as rainfall-runoff (RR) hydrological model has become a useful tool which can significantly improve efficiency of the hydropower energy generation, water supply management, and agricultural irrigation water utilization. The accuracy and reliability of the water quantity simulation & forecasting model are significantly affected by the model parameters. Therefore, demand of effective and fast model parameter optimization tool for solving the E-W-F nexus problem increases significantly. The shuffled complex evolution developed at University of Arizona (SCE-UA) has been recognized as an effective global model parameter optimization method for more than 20 years and is highly suited to solve the E-W-F nexus problem. However, the computational efficiency of the SCE-UA dramatically deteriorates when applied to complex E-W-F nexus problem. For the purpose of solving this conundrum, a fast parallel SCE-UA was proposed in this paper. The parallel SCE-UA was implemented on the novel heterogeneous computing hardware and software systems which were constituted by the Intel multi-core CPU, NVIDIA many-core GPU, and PGI Accelerator Visual Fortran (with OpenMP and CUDA). Performance comparisons between the parallel and serial SCE-UA were carried out based on two case studies, the Griewank benchmark function optimization and a real world IHACRES RR hydrological model parameter optimization. Comparison results indicated that the parallel SCE-UA outperformed the serial one and has good application prospects for solving the water quantity simulation & forecasting model parameter calibration in the E-W-F nexus problem.

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1. Introduction

With continuous population increase and economic growth, challenges on securing sufficient energy, water, and food supplies to meet the demand are amplifying significantly. The close linkages of the three sectors give rise to the need for tackling the challenges with a nexus approach. Information shared and interpreted jointly between these three sectors is important for better understanding the complicity of the energy-water-food (E-W-F) nexus and taking integrated approaches for their management [1–3]. Among these three sectors, water plays the most important role in the E-W-F nexus issue such as energy supply (clean hydropower energy generation), water supply (drinking water), and food supply (agricultural irrigation water). Water quantity simulation & forecasting significantly affect the energy and food utilization & management in E-W-F nexus issue. For example, in the field of hydropower energy generation and management, we cannot generate and manage the electricity appropriately without the accurate inflow forecasting information. With an accurate inflow forecasting report, we can dispatch the hydropower plant to generate electricity and conserve energy more efficient. Additionally, with the exacerbation of the nature resources depletion and climate change, better theoretical, methodological, and empirical technologies for solving the complex water quantity simulation & forecasting problem in the E-W-F nexus issue is in great need [4–9]. Water quantity simulation & forecasting model, such as rainfall-runoff (RR) hydrological model, has been proved to be a useful tool for solving the problems encountered in the E-W-F nexus issue. RR hydrological models, such as the IHACRES model, etc., have been successfully applied to assist the solution of the E-W-F nexus issue [10–12].

The RR hydrological models have been more and more popular nowadays, and provide researchers and engineers powerful tools for solving the E-W-F nexus issues. Among key points for obtaining good simulation and forecasting results, the determination of the model parameters plays a significantly important role. Without properly optimized model parameters, the model performance will be dramatically deteriorated. With the development of computational mathematics and computer science & technology, computer-based automatic parameter optimization method has become a widely used tool in the field of model parameter calibration and system identification [13–21]. The typical automatic optimization methods include genetic algorithm, particle swarm optimization, and differential evolution. However, in the complex real world applications such as water quantity simulation and forecasting model calibration for E-W-F nexus issue, these methods show some disadvantages such as poor optimization accuracy, non-global optimality, and instability. These problems have been solved by an effective and robust global optimization method, shuffled complex evolution developed at University of Arizona (SCE-UA) [22–27]. The SCE-UA method combines the concept of combination of deterministic and stochastic optimization [28], competitive evolution [29], and sub-population information sharing [30]. The effectivity, robustness, and stability of the SCE-UA method have been widely verified by a large number of researches and real world applications. The SCE-UA method has been successfully applied in the water quantity simulation and forecasting model parameter optimization tasks and is highly suited to solve the E-W-F nexus problem.

2. The deficiency of the SCE-UA and the motivation of this research

Although the SCE-UA method has been successfully applied in many researches and engineering applications, its low computational efficiency for highly complex applications, such as RR hydrological model parameter calibration in the E-W-F nexus issue, has become a conundrum which limits its further use. The SCE-UA method searches the global optimum according to the information provided by the objective function value which is computed by running the hydrological model repeatedly. Generally, the computational load of the hydrological model run is very high. For complex E-W-F nexus optimization problem, SCE-UA should generate large number of complexes and should carry on large number of objective function evaluations to ensure the global optimality of the final solution. These factors make the optimization process more complex and will consume much more computation resources, and therefore dramatically slowdown the convergence speed. The original serial computation program runs too slow and cannot satisfy the requirement of fast model parameter calibration for the E-W-F nexus optimization problem.

The best way to boost the computational efficiency of the scientific computing is the use of the modern hardware acceleration technology. There are two kinds of acceleration technologies combined together to form the nowadays famous "heterogeneous computing" hardware acceleration technology. They are multi-core CPU and many-core GPU acceleration technologies [31–34]. A multi-core central processing unit (CPU) is a single computing component with two or more independent actual processing units (called "cores"), which are the units that read and execute program instructions. The instructions are ordinary CPU instructions (such as add, move data, and branch), but the multiple cores can run multiple instructions at the same time, increasing overall speed for programs amenable to parallel computing. Manufacturers typically integrate the cores onto a single integrated circuit die (known as a chip multiprocessor or CMP), or onto multiple dies in a single chip package. GPU is referred to as graphics processing unit, which is originally used for pictures and videos processing. Pioneered in 2007 by NVIDIA Corporation, the GPU was introduced to the general purpose computing (GPGPU) and run much faster than traditional multi-core CPU. GPU-accelerated computing is the use of a GPU together with a CPU to accelerate scientific, analytics, engineering, consumer, and enterprise applications. NVIDIA GPU accelerators now power energy-efficient datacenters in government labs, universities, enterprises, and small-and-medium businesses around the world. GPUs are accelerating applications in platforms ranging from cars, to mobile phones and tablets, to drones and robots [35–37]. A simple way to understand the difference between a CPU and GPU is to compare how they process tasks. A CPU consists of a few cores optimized for sequential serial processing or low intensive parallel processing while a GPU has a massively parallel architecture consisting of thousands of smaller, more efficient cores designed for handling multiple highly parallel tasks simultaneously. Heterogeneous computing offers unprecedented application performance by assigning logical-intensive and compute-intensive portions of the application to the CPU and GPU, respectively. From a user's perspective, applications simply run significantly faster. The heterogeneous computing technology is highly suited to the acceleration of the SCE-UA method. However, little previous literatures reported the heterogeneous computing accelerated SCE-UA and this is a completely novel research field.

In order to accelerate the SCE-UA method for fast RR hydrological model parameter optimization in E-W-F nexus problem, the original serial method was analyzed and was properly parallelized. And then, the parallel SCE-UA method was implemented on the recently emerging heterogeneous computing hardware and software systems, which are constituted by Intel multi-core CPU, NVIDIA many-core GPU, and PGI Accelerator Visual Fortran (with OpenMP and CUDA). Based on the Griewank benchmark function and a real world RR hydrological IHACRES model, the performance comparisons were studied. The comparison results indicated that