21st International Congress on Modelling and Simulation, Gold Coast, Australia, 29 Nov to 4 Dec 2015
www.mssanz.org.au/modsim2015

# Development of a parallel computing enabled optimisation tool for hydrological model calibration

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**Abstract:** A river model is a semi-distributed hydrological model and it includes many processes such as flow routing, irrigation diversion, overbank flow, ground water interaction for simulating flows a river system for water resources planning and management. A number of calibration parameters are introduced in such models to represent various processes using simplified mathematical equations. Traditionally, a river model is calibrated using a reach-by-reach calibration approach starting from the top of the system cascading down to the end of the system. While the reach-by-reach approach is suitable for obtaining optimum model performance at a single river reach with high quality observed data, it does have the limitation of error propagation from upstream to downstream reaches if poor quality data are used in the calibration. A system-wide calibration approach has recently been developed for river system modelling in large river basins. Comparing with traditional reach-by-reach calibration, this new method optimises parameters of all river reaches within a region simultaneously using a weighted global objective function. The results of its application of this new approach in the Murray-Darling basin, Australia have shown its potential to overcome over-fitting and improve fitness of each individual gauge. However, due to the system-wide optimization of multiple reach parameters in a region, the search space and computational time required for system calibration increase exponentially with the increase of number of parameters. This limits the number of parameters that can be optimised and thus, the size of the region. To potentially overcome this limitation, a parallel computing enabled shuffled complex evolution (SCE) optimisation tool has been developed. A series of comparison studies have been conducted to evaluate the performance of this approach over normal SCE. These are: 1) comparison of computation time and performance for the same number of parameters; 2) comparison of performance with the same computation time and the same number of parameters and 3) comparison of the maximum number of parameters that can be optimised and performance within the same computation time. The results show that the run time with the new approach is about 25% of those with the normal SCE and its efficiency increases with increased number of calibration parameters.

***Keywords:*** *River system model, Australian Water Resources Assessment, Shuffled complex evolution, parallel computing, optimisation*

## 1. INTRODUCTION

A river model is a semi-distributed hydrological model designed for simulating flows in regulated and un-regulated river systems and is widely used by the state and federal water agencies across Australia for water resource assessment, planning and policy making. A regulated river system model includes many processes such as flow routing, irrigation diversion, overbank flow, ground water interaction. Various river models have been developed and used by different agencies for water resource assessment, planning and policy making (Welsh et al., 2013). One of such river models is the Australian Water Resource Assessment (AWRA) River model (AWRA-R), which has been recently developed by CSIRO in alliance with the Australian Bureau of Meteorology (BoM). The core objective of the AWRA-R model is to simulate various fluxes and stores associated with a river system to enable BoM to produce national water accounts.

In a river system model, a number of calibration parameters are introduced in the model to represent various processes using simplified mathematical equations. For example, AWRA-R model includes 8 parameters. Calibration of such model parameters is a critical step to enable a river system model to simulate the behavior of a real world system as close to the observation as possible. However, such calibration of a river model with a large number of calibration parameters is computationally intensive. Therefore, a reach-by-reach calibration is typically used to calibrate most of the river system models, where Each reach or gauge in a river system is calibrated separately in a cascading manner from upstream to downstream reaches (Lerat et al., 2013). In such a way, only parameters within the same reach are calibrated at a time. In this approach, calibration errors, i.e. over-fitting to poor gauge data, propagate to downstream. In turn, it introduces water balance error and reduces goodness of fit at downstream gauges (Hughes et al., 2014a). To overcome this problem, Hughes et al. (2014b and 2015) proposed a system-wide calibration approach, in which all reaches or gauges within a modelling domain are calibrated simultaneously using a weighted system objective function for all stream flow gauges. Weight is assigned to each gauge in the system based on its magnitude and quality of available data. Its application to Murrumbidgee catchment (Hughes et al. 2014b and 2015) showed that the system calibration approach provided an overall improved goodness-of-fit by reducing the propagation of calibration error from upstream to downstream. The shuffled complex evolution (SCE-UA) (Duan et al., 1992 and 1993), as a robust and efficient search algorithm, was used as the optimizer in the system calibration. By its nature of evolutionary algorithm, the computational time increases exponentially with increase of the number of calibrated parameters. This limits the system calibration to be applied into large regions.

To overcome above limitation, a parallel computing enabled shuffled complex evolution (PCE-SCE) system calibration tool has been developed and implemented for system-wide calibration of AWRA-R model parameters for different regions/sub-regions within the Murray-Darling Basin (MDB). The results demonstrate that the PCE-SCE is more efficient than the SCE-UA, especially for calibrating a large number of parameters.

This paper has introduced the new PCE-SCE tool and its application in the MDB. The SCE-UA is briefly introduced in the next section, followed by a detailed description of the proposed PCE-SCE. The results from a series experiments in the MDB are then presented and discussed. The final section presents the conclusions drawn from the study.

## 2. THE SCE-UA

The SCE-UA was originally developed at the University of Arizona (Duan et al. 1992 and 1993) in order to effectively and efficiently calibrate high dimensional conceptual rainfall-runoff models. This method is derived from genetic algorithm and integrates the best features of the new concept of complex shuffling and three existing techniques, including combination of probabilistic and deterministic strategies, clustering and competitive evolution (Holland 1975, 1983; Manetsch, 1990; Wang, 1991). In general, there are six steps in the SCE-UA:

1. Generate initial population – if there is no prior knowledge, just use a uniform probability distribution to generate predefined number of solutions within the feasible solution space, then evaluate them against predefined objective function and calculate their fitness;
2. Rank each individual solution – sort all solutions within the population in ascending order according to their fitness (assuming that the goal is to minimize the fitness);
3. Partition into complexes – the generated solutions are partitioned into a number of complexes, each of which has the same size of solutions;
4. Evolve each complex – each complex is evolved independently for a predefined number of times according to the competitive complex evolution algorithm, which is based on the simplex downhill search method (Nelder and Mead, 1965). A simplex or sub-complex is generated from the complex according to a

trapezoidal probability distribution. The simplex then evolves with the three types of evolutionary techniques: reflection, contraction and mutation.

The worst solution of the simplex is first identified and reflected through the centroid of the simplex without the worst solution.

a) If the new reflected solution is out of the feasible solution space, it will use mutation technique to randomly generate a new solution within the feasible solution space;
b) If the new reflected solution is within the feasible solution space and better than the worst solution, it will replace the worst solution. Otherwise, a contraction step is taken by computing a solution halfway between the worst solution and the centroid of the simplex without the worst solution. If this new contraction solution is better than the worst solution, it will replace the worst solution. Otherwise a new solution is randomly generated by using mutation technique.

The number of times to generate a simplex is predefined and the number of steps taken within the simplex is also predefined.

5. Shuffle all complexes – combine all complexes together to a single population;
6. Check convergence or stop criteria – if any of the predefined convergence criteria or stop criteria is satisfied, stop. Otherwise go to step 2.

## 3. THE PCE-SCE

It is obvious that the step 4 in the above algorithm is the core of SCE-UA and high computationally intensive. Fortunately, this step also shows its high independency that all complex is evolved totally independent from each other. This independency makes it to be natural to evolve each complex in parallel. The proposed PCE-SCE is designed by taking advantage of this independency to optimize computational efficiency by parallelizing step of SCE-UA. In this approach, the complexes are evolved in parallel, on different CPU cores instead of a single CPU core. After the population is partitioned to complexes, the complexes are sent to and evolved independently on different CPU cores. The evolved complexes are then sent back to the main CPU core where all complexes are shuffled into a single population. If convergence or stop criteria are not met, solutions are ranked, the population is partitioned into complexes again and a new loop starts. The brief algorithm of the PCE-SCE is shown in Figure 1. To demonstrate its performance and how it works, a series experiments are conducted in the MDB and described in the following section.

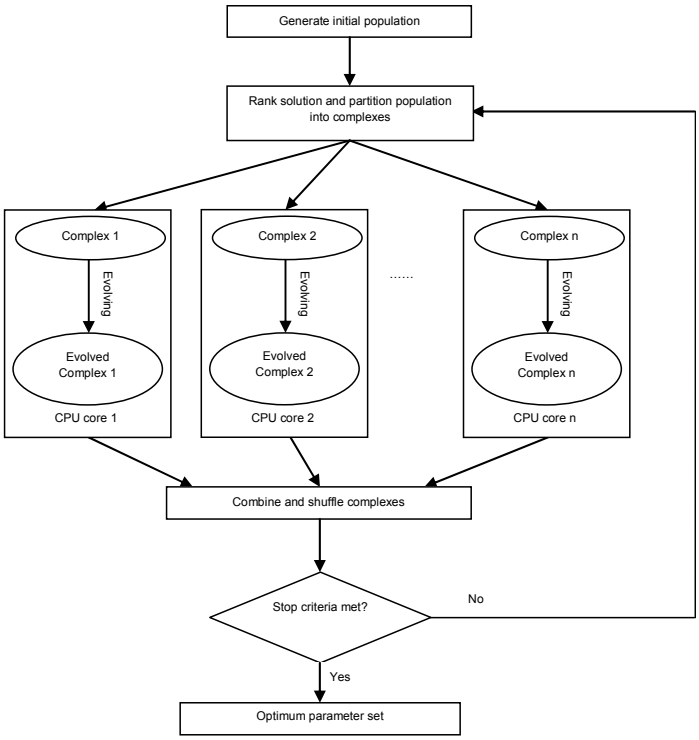


**Figure 1.** Algorithm of the PCE-SCE.

## 4. EXPERIMENTS

The PCE-SCE is implemented in R and tested on the CSIRO Accelerator Cluster Bragg that consists of 128 Dual Xeon 8-core E5-2650 Compute Nodes (i.e. a total of 2048 compute cores) with 128 GB of RAM, 500 GB SATA storage and FDR10 InfiniBand interconnect. All river models in the MDB are calibrated by both the PCE-SCE and the SCE-UA with the same configuration. The performance and running time from each algorithm are then compared and analysed.

### 4.1. AWRA-R model

The river model AWRA-R in the Australian Water Resource Assessment (AWRA) modelling system is adopted as the modelling tool in this study. Like other river system models, AWRA-R model attempts to simulate natural hydrological process and human activities of water diversion infrastructures (e.g. dams, canal intakes, pumps, etc.) within a river reach. The AWRA-R is a node-link based model, where a river system is schematised into a simplified river network for routing flows along a river system at a daily time step (Welsh et al., 2013). The current version of the AWRA-R model (version 5.0) consists of 10 components (Dutta et al., 2015): Streamflow routing, Local ungauged runoff, Storage contribution modelling, Irrigation modelling, Urban water use, Water use for stock and domestic, Rainfall to and evaporation from river, Anabranch flow, Floodplain inundation modelling, River and groundwater interaction modelling and Head-water catchment modelling. Figure  shows a conceptual diagram of a river reach (in a residual catchment) with different components of the model. In an AWRA-R simulation of a reach, all upstream inflows are routed first and then, local inflows are added and losses are subtracted to calculate the outflow at the end of the reach. The general form of water balance for a reach (with routed upstream flow) for AWRA-R v5.0 can be described as follows:

$$\widehat{Q_{d/s}} = (Q_{u/s})_{rout} + Q_r + Q_s - Q_d + Q_{irr} - Q_u - Q_{sd} + Q_p - Q_e - Q_a - Q_{fp} + Q_{fpr} - Q_{gw}$$

Where, $\widehat{Q_{d/s}}$: simulated flow at the downstream gauge (m3/sec), $Q_{u/s}$: concurrent flow at the upstream gauges (including gauged tributaries) (m3/sec), $(Q_{u/s})_{rout}$: upstream inflow following routing (m3/sec), $Q_r$ : runoff locally generated from the local ungauged catchment (m3/sec), $Q_s$ : contribution from any storages including rainfall on storage area, evaporation from storage area and change in storage volume (m3/sec), $Q_d$ : loss due to irrigation diversion (m3/sec), $Q_{irr}$ : total return flow from irrigated area (m3/sec), $Q_u$ : net loss due to urban diversion (m3/sec), Qsd : rural water use (other than irrigation) for stock and domestic (m3/sec), $Q_p$ : the flux to the river store due to rainfall (m3/sec), $Q_e$ : the flux from the river due to evaporation (m3/sec), $Q_a$: the flow diverted to anabranches (m3/sec), $Q_{fp}$= overbank flow to floodplain (m3/sec), $Q_{fpr}$: return flow from floodplain (m3/sec),and $Q_{gw}$: the flux from river to groundwater (m3/sec).

AWRA-R model has 8 calibration parameters for every modelled reach: *Lag, K, x, OT, FR, $M_1$, $M_2$, SF* (Dutta et al., 2015). The first three parameters (*Lag, K, x)* are associated flow routing from upstream to downstream using Muskingum routing scheme. Parameters *OT* (overbank flow threshold) and *FR* (floodplain return flow coefficient) are associated with overbank flow modelling component (Dutta et al., 2013). $M_1$ and $M_2$ are two parameters of MONOD function, which is used to constraint groundwater recharge estimate from a river reach (Dutta et al., 2015). The final parameter (*SF*) is a scaling factor used for scaling the ungauged runoff obtained from AWRA-L model.

### 4.2. Study area

The study area in this paper consists of 18 reporting regions (Figure 2. The conceptual diagram of AWRA-R reach**.** Figure ) in the MDB basin as in the MDB sustainable yield project (CSIRO 2008). Due to the size, some regions are divided into two sub-regions. Therefore, in total there are 22 region/sub-regions, each of which is modeled by an AWRA-R model.

## 5. MODEL CALIBRATION

In the model calibration, all parameters are calibrated reach-by-reach first (Lerat et al, 2013), and then followed by a system-wide calibration for each region/sub-region in the MDB. The optimum parameter sets found in the reach-by-reach calibration are used as the initial parameter set in the system calibration. In the system calibration, 4 parameters related to reach losses and gains are selected from each reach. They are: ungauged inflow correction factor, flood plain return flow coefficient and GW loss (α and β). All selected parameters for all reaches within a region or sub-region are calibrated simultaneously by the PCE-SCE and the SCE-UA, respectively.

The objective function used for each reach is a combination of daily Nash-Sutcliffe efficiency (Nash and Sutcliffe 1970) with root transformed values and a bias given by:

$$OF = \left(1 + \frac{\sum\left(\sqrt{Q_i^s} + \sqrt{Q_i^o}\right)^2}{\sum(\sqrt{Q_i^o} - \overline{\sqrt{Q^o}})^2}\right) * \left(1 + \left|\frac{\sum Q_i^s - \sum Q_i^o}{\sum Q_i^o}\right|\right)$$

Where $OF$ is the objective fitness, $Q^s$ is the simulated stream flow daily time series, $Q^o$ is the observed stream flow daily time series. The bias $\left|\frac{\sum Q_i^s - \sum Q_i^o}{\sum Q_i^o}\right|$ is introduced in the objective function to ensure that the total modelled stream flow matches the total observed stream flow. The function is minimized in the calibration and the $OF$ will be 1 if the simulated stream flow perfectly match the observed stream flow. The higher the $OF$, the poorer the fit.

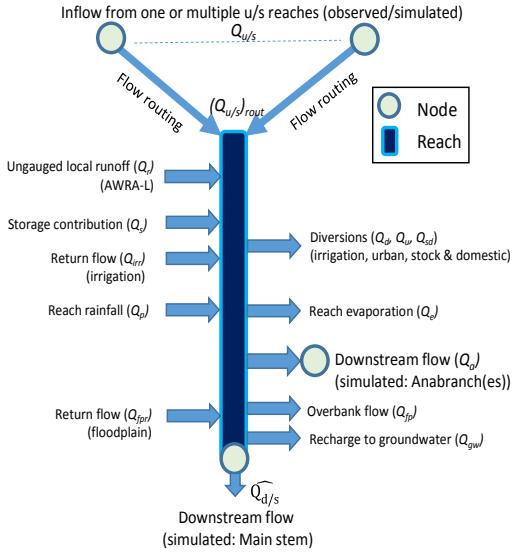


**Figure 2.** The conceptual diagram of AWRA-R reach.


**Figure 3.** Reporting regions in the MDB.

The overall objective fitness of a region in the system calibration is a weighted sum of the objective fitness of all reaches within the region given by:

$$OF_{sys} = \sum W_j * OF_j$$

Where, $OF_{sys}$ is the overall system objective fitness for a region/sub-region, $OF_j$ is the objective fitness of a gauge in the region/sub-region and $W_j$ is the weight of a gauge. Given the importance of mean flow rate and length of observed record, the $W_j$ is calculated as:

$$w_j = \frac{\sum_{i=1}^{m} Q_{i,j}}{\sum_{j=1}^{n}\sum_{i=1}^{m} Q_{i,j}}$$

Where, $w_j$ is the weight for the gauge $j$, and $Q_{i,j}$ is the observed stream flow for the gauge $j$ on the day $i$. The sum of all gauge weights should be 1.

## 6. RESULTS AND DISCUSSION

Each system calibration includes 5 replicates with different seeds and runs at a daily time-step from 1/1/1970 to 30/06/2014. The total number of parameters calibrated in the system calibration varies from 8 (Moonie) to 84 (Macquarie-Castlereagh Bottom sub-region) (see Figure 4).

The overall system objective fitness $OF_{sys}$ of the best solution for each region/sub-region found by the PCE-SCE and SCE-UA is shown in Figure 4. Since search algorithm is the same, it is not surprised to see that the best $OF_{sys}$ found by the PCE-SCE and the SCE-UA is much similar across all regions/sub-regions. However the run times used by the PCE-SCE are much reduced compared to the SCE-UA for all regions/sub-regions as shown in Figure 5. Both figures also suggest that the run time and the number of parameters follow a power law. According to this relationship, the average running time used by the PCE-SCE is about 25% of that by the SCE-UA if less than 50 parameters are calibrated. For calibrating more than 50 parameters, the PCE-SCE saves even more time. The average running time is about 21% of that by the SCE-UA if 50 to 80 parameters are calibrated.

The run time for calibrating the same number of parameters varies between replicates for both cases. The variance increases with the increased number of parameters. Sometimes the running time of one replicate is more than double of another replicates. It indicates that the solution space is very rugged and the starting point is critical to the searching process in the SCE. If 5 days (120 hrs) is the maximum acceptable running time, the SCE-UA can only handle the model with less than 50 parameters while the PCE-SCE can handle up to 80 parameters. This is the reason why 4 regions have to be divided into two sub-regions.

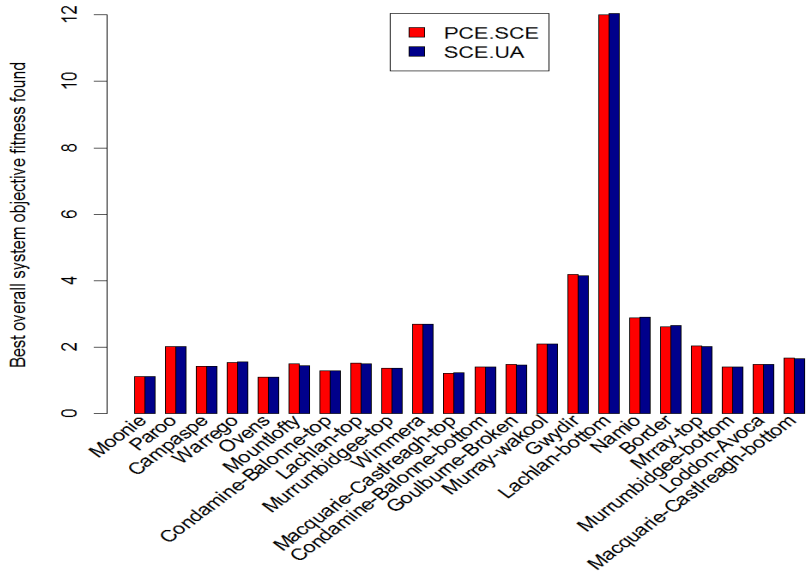


**Figure 4.** $OF_{sys}$ of the best solution found by the PCE-SCE and the SCE-UA.

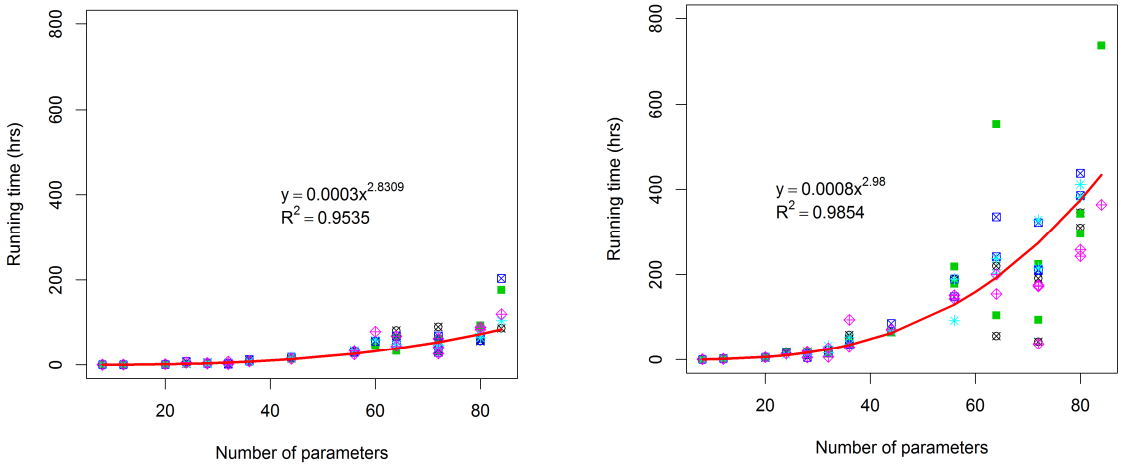


**Figure 5.** Run time vs. number of parameters by the PCE-SCE (left) and the SCE-UA (right).

## 7. CONCLUSION

This paper proposed a parallel computing enabled SCE optimizer, which has been used to calibrate AWRA-R river system model in 22 regions/sub-regions within the MDB. The run time of calibrating the same number of parameters with the same configurations is largely reduced by using the PCE-SCE when comparing with the SCE-UA (up to about 25%). The efficiency of PCE-SCE increases with increased number of calibration parameters. Within the same run time, a much better solution is found by the PCE-SCE than the SCE-UA. However, this study also shows some limitations of the PCE-SCE. For example, the search process is directly impacted by the starting point, especially for calibration of a large number of parameters. The running time and its variance between replicates becomes unacceptable when calibrating a large number of parameters, e.g. more than 80 parameters. There is a scope for further investigation to overcome that.

**ACKNOWLEDGEMENT**

The authors are grateful to CSIRO and the Bureau of Meteorology for funding this work under the WIRADA research alliance.

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