



## **A Parallel Simulation-Optimization Framework for Efficient Calibration of Computationally Expensive Urban Reservoir Hydrodynamic and Water Quality Models**

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Process-based numerical models are frequently used by policymakers and water managers for decision-support in effective water quantity and quality management of urban water system reservoirs and lakes. Such models (e.g., Delft3D hydrodynamic and water quality models) typically involve systems of partial differential equations and are highly parameterized and expensive to compute. Hence, extensive human and computational effort for parameter calibration are required. Recent studies have demonstrated that High-Performance Computing (HPC) and efficient optimization techniques can be effective in automatic calibration and scenario optimization of computationally expensive environmental models. This study applies a parallel surrogate-assisted global optimization method within a simulation-optimization framework for efficient automatic calibration of computationally expensive lake hydrodynamic and water quality models. The simulation-optimization framework is implemented generically for Delft3D hydrodynamic and water quality models, and can also be applied to water quality planning and management optimization formulations. We apply our parallel framework for i) calibration of water temperature for a computationally expensive reservoir Delft3D hydrodynamics model (Delft3D-FLOW) and ii) multi-constituent (Chlorophyll-A, Total Nitrogen and Total Phosphorus) calibration of a reservoir Delft3D water quality model (Delft3D-WAQ). Both Delft3D models solve lots of partial differential equations and are expensive to compute. A single 1-year simulation of the hydrodynamics model with time step 1.5 minutes takes 4 to 5 hours on a Windows desktop with CPU Intel Core i7-4790. The reservoir water quality model requires 15-20 minutes for simulating given input from the hydrodynamics model. We ran our parallel calibration experiments on ASPIRE1 which is Singapore's first petascale supercomputer. Results indicate that our simulation-optimization framework performs considerably better and require significantly less computational and human effort (order of days) than manual calibration. A key purpose of this study is to illustrate (to policymakers and water managers) that efficient parallel surrogate-assisted simulation-optimization frameworks can be effectively used to calibrate the computationally expensive Delft3D models developed for Singapore's urban reservoirs with relatively few model evaluations. In future we plan to run these algorithms on Delft3D models asynchronously to further improve computational efficiency.