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hydroPSO: A Versatile Particle Swarm Optimisation R Package for Calibration of Environmental Models

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Particle Swarm Optimisation (PSO) is a recent and powerful population-based stochastic optimisation technique inspired by social behaviour of bird flocking, which shares similarities with other evolutionary techniques such as Genetic Algorithms (GA). In PSO, however, each individual of the population, known as *particle* in PSO terminology, adjusts its *flying trajectory* on the multi-dimensional search-space according to its own experience (best-known *personal* position) and the one of its neighbours in the swarm (best-known *local* position). PSO has recently received a surge of attention given its flexibility, ease of programming, low memory and CPU requirements, and efficiency. Despite these advantages, PSO may still get trapped into sub-optimal solutions, suffer from swarm explosion or premature convergence. Thus, the development of enhancements to the "canonical" PSO is an active area of research. To date, several modifications to the canonical PSO have been proposed in the literature, resulting into a large and dispersed collection of codes and algorithms which might well be used for similar if not identical purposes.

In this work we present *hydroPSO*, a platform-independent R package implementing several enhancements to the canonical PSO that we consider of utmost importance to bring this technique to the attention of a broader community of scientists and practitioners. *hydroPSO* is model-independent, allowing the user to interface any model code with the calibration engine without having to invest considerable effort in customizing PSO to a new calibration problem. Some of the controlling options to fine-tune *hydroPSO* are: four alternative topologies, several types of inertia weight, time-variant acceleration coefficients, time-variant maximum velocity, regrouping of particles when premature convergence is detected, different types of boundary conditions and many others. Additionally, *hydroPSO* implements recent PSO variants such as: Improved Particle Swarm Optimisation (IPSO), Fully Informed Particle Swarm (FIPS), and weighted FIPS (wFIPS). Finally, an advanced sensitivity analysis using the Latin Hypercube One-At-a-Time (LH-OAT) method and user-friendly plotting summaries facilitate the interpretation and assessment of the calibration/optimisation results.

We validate *hydroPSO* against the standard PSO algorithm (SPSO-2007) employing five test functions commonly used to assess the performance of optimisation algorithms. Additionally, we illustrate how the performance of the optimization/calibration engine is boosted by using several of the fine-tune options included in *hydroPSO*. Finally, we show how to interface SWAT-2005 with *hydroPSO* to calibrate a semi-distributed hydrological model for the Ega River basin in Spain, and how to interface MODFLOW-2000 and *hydroPSO* to calibrate a groundwater flow model for the regional aquifer of the Pampa del Tamarugal in Chile. We limit the applications of *hydroPSO* to study cases dealing with surface water and groundwater models as these two are the authors' areas of expertise. However, based on the flexibility of *hydroPSO* we believe this package can be implemented to any model code requiring some form of parameter estimation.