

A Surrogate Based Optimization Approach for the Development of Uncertainty-Aware Reservoir Operational Rules: the Case of Nestos Hydrosystem

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Received: 22 October 2014 / Accepted: 2 August 2015 © Springer Science+Business Media Dordrecht 2015

Abstract Operation of large-scale hydropower reservoirs is a complex problem that involves conflicting objectives, such as hydropower generation and water supply. Deriving optimal operational rules is a challenging task due to the non-linearity of the system dynamics and the uncertainty of future inflows and water demands. A common approach to derive optimal control policies is to couple simulation models with optimization algorithms. This paper in order to investigate the performance of a future reservoir and safely infer about its significance employs stochastic simulation, thus long synthetically generated time-series and a multi-objective version of the Parameterization-Simulation-Optimization (PSO) framework to develop uncertaintyaware operational rules. Furthermore, in order to handle the high computational effort that ensues from that coupling we investigate the potential of a surrogate-based multiobjective optimization algorithm, ParEGO. The PSO framework is deployed with WEAP21 water resources management model as simulation engine and MATLAB for the implementation of optimization algorithms. A comparison between NSGAII and ParEGO optimization algorithms is performed to assess the effectiveness of the proposed algorithm. The aforementioned comparison showed that ParEGO provides efficient approximations of the Pareto front while reducing the computational effort required. Finally, the potential benefit and the significance of the future reservoir is underlined.

Keywords Multi-objective optimization under uncertainty \cdot Surrogate based optimization \cdot Hydrosystem management \cdot Hydro-energy \cdot WEAP21 model

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1 Introduction

A hydrosystem is defined as a system consisting of natural water bodies and technical projects whose collaboration serves one or more purposes. To serve these purposes it is necessary to analyze the hydrosystem and identify optimal management policies. The operation of a reservoir system involves a complex decision making process, many variables and objectives, as well as risk and uncertainty (Oliveira and Loucks 1997). Detailed release policies for each reservoir in a system can be derived with the use of simulation models and optimization tools. Optimizing water management strategies is complex, as some impact relationships are non-linear and interdependent (Vink and Schot 2002).

The involved conflicting objectives make the problem multi-objective. Therefore, there is no unique optimal solution. Instead, the interaction of multiple objectives yields a set of efficient, known as Pareto-optimal solutions, which give the decision maker more flexibility in the selection of suitable alternatives. Additionally, the explicit investigation of the objectives' tradeoff provides a valuable tool to decision makers (Makropoulos and Butler 2005). Problems that involve multiple objectives can be addressed by the coupling of simulation models and multi-objective evolutionary optimization (MOEA) algorithms (Nicklow et al. 2010). Such schemes and frameworks have been widespread and popular within water resources scientific community and extensive reviews can be found in literature (e.g., Efstratiadis and Koutsoyiannis 2010; Nicklow et al. 2010; Reed et al. 2013). On the other hand when dealing with real-world applications where computational time is often limited, the number of iterations, the large decision space, the complexity of the fitness landscape and the long simulation time required by the simulation models consists major drawbacks.

As far it concerns hydrosystem optimization and thus derivation of optimal operational rules the robustness and the effectiveness of such rules is significantly affected by hydrological uncertainties and climate variability. One way to address this issue is the use of stochastic simulation within the simulation-optimization process (Koutsoyiannis 2000, 2005); i.e., the generation and use of synthetic time-series. This way risk-based and robust operational rules that encapsulate the hydrological variability can be derived. The synthetic time-series are generated using stochastic models that are able to reproduce the statistical properties of historical data. However the use of long synthetic time-series drastically increases the computational effort required and thus imposes a limit in their practical application.

This work employs a recently presented multi-objective version (Tsoukalas and Makropoulos 2014) of Parameterization-Simulation-Optimization (PSO) framework which was originally (in single-objective formulation) proposed by Koutsoyiannis and Economou (2003). PSO is capable of deriving uncertainty-aware reservoir operation rules through the use of stochastic simulation. The advantages of the latter over other similar methods (such implicit stochastic optimization (ISO) and explicit stochastic optimization (ESO)) are the parsimonious parameterization, the incorporation of hydrological uncertainty and the simplicity of the operational rules that provide. The latter is essential in order to bridge the gap between research developments and real-world applications (e.g., Celeste and Billib 2009; Labadie 2004; Simonovic 1992; Yeh 1985).

The integrated model is consisted by WEAP21 water resources management model (Yates et al. 2005) where the simulation part is performed and MATLAB where the optimization part is implemented. This way the capabilities of the model have been extended by using it within PSO framework (named WEAP21-PSO). The methodology is demonstrated in the especially challenging, trans-boundary hydrosystem of Nestos, shared between Greece and Bulgaria.

Within the same context different infrastructure scenarios are explored in order to preliminary assess and quantify the contribution of a future hydropower reservoir to the overall hydrosystem.

Additionally, in order to ensure the computational practicability of PSO and overcome the bottleneck posed by the use of long synthetic time-series we employ a multi-objective surrogate based optimization (SBO) algorithm, namely ParEGO (Knowles 2005). Furthermore, in order to validate ParEGO efficiency prior to its employment within PSO framework a preliminary comparison with the well-known NSGAII (Deb et al. 2002) is performed using historical data.

2 Methodology

2.1 Methodology Overview

The main tools used in this study were; WEAP21¹ water resources management model (Yates et al. 2005) to simulate the hydrosystem and MATLAB as an environment for the implementation of the optimization algorithms. In this study a bespoke code handling the interaction between the two programs was developed in MATLAB, using the COM-API² available in WEAP21. That interaction makes possible a bi-directional cooperation between WEAP21 and MATLAB, enabling a two-way communication between the simulation and optimization models through the COM-API capabilities of WEAP21 as discussed in Tsoukalas and Makropoulos (2013).

In order to develop uncertainty-aware operational rules and investigate the potential of a future reservoir this paper employs a multi-objective version of PSO framework. The basic steps of PSO (Koutsoyiannis and Economou 2003) are: 1) Representation of the main hydrological components (i.e., precipitation, evapotranspiration, inflow) through stochastic simulation, using stochastic simulation models that generate long synthetic time-series able to capture and reproduce the statistical properties of the historical sample. 2) Parsimonious parameterization of the operational rule (management policy) of the reservoir system using as small number of decision variables θ . 3) Definition of appropriate objective function(s) that express the desired performance metric(s). 4) Simulation of the hydrosystem using the synthetic time-series to drive the simulation and implementing the parameters that define the management policy. 5) Utilization of an optimization algorithm to derive the best managerial policy.

The stochastic simulation of hydrological variables (step 1) was performed with the use Castalia software³ (Efstratiadis et al. 2014). Castalia is a multivariate stochastic simulation model developed for the study of monthly and daily hydrological variables such as rainfall, evapotranspiration and inflow. It generates synthetic time-series on the basis of historical data, that preserve and reproduce the statistical properties, including mean value, standard deviation, skewness, autocorrelation and cross-correlation of the observed data sets (Efstratiadis et al. 2005). Another key element of Castalia is that reproduces the long-term persistence of hydrological processes, also known as Hurst-Kolmogorov dynamics (Koutsoyiannis 2011),

¹ http://www.weap21.org

² Component Object Model Application Programming Interface

³ http://www.itia.ntua.gr/en/softinfo/2/

in both annual and inter-annual scale, as well as the periodicity in infra-annual scale and intermittent behavior on daily scales.

In order to express the operational rules it is essential to determine suitable control variables θ and performance measures (objective functions). Regarding parameterization of the operational rules of the hydrosystem (step 2), a parsimonious approach is implemented; each reservoir was parameterized by 3 variables (θ_1 , θ_2 , θ_3) referring to energy production targets for different months. For *n* reservoir there is a parameter θ_{1n} referring to December and January, is a parameter θ_{2n} referring to May and September and a parameter θ_{3n} referring to June, July and August. The interim values referring to energy production targets were calculated with linear interpolation.

Regarding the performance criteria (step 3), three objective functions were introduced (*Y1*, Υ 2 and Υ 3). All of them are based on the monthly time-series of hydropower production $E_i(t)$ of each hydropower reservoir *n*. The first one is constant monthly firm energy maximization for given reliability level *a* (i.e., a=99%). The energy produced above firm is called secondary or excessive energy. (e.g., Efstratiadis et al. 2012; Hamlet et al. 2002; Larson and Larson 2007).

$$Y1(\boldsymbol{\theta}) = f\left(\sum_{i=1}^{n} E_i(t)\right) \tag{1}$$

Monthly firm energy is the guaranteed energy produced from the hydropower reservoirs for certain reliability level.

The second criterion is the maximization of the weighted sum of the average monthly energy.

$$Y2(\boldsymbol{\theta}) = \left\{ \sum_{j=i}^{12} mean \left[w_j(t) \sum_{i=1}^n E_i(t) \right] \right\}$$
(2)

And finally the third one is the maximization of the weighted sum of the monthly firm energy for given reliability a.

$$Y3(\boldsymbol{\theta}) = \left\{ \sum_{j=i}^{12} f\left[w_j(t) \sum_{i=1}^n E_i(t) \right] \right\}$$
(3)

where, *f* denotes to the firm energy of the system estimated on the basis of hydropower production $E_i(t)$ and *n* is the number of hydropower plants. The firm energy is calculated as the desired reliability *a* for hydropower production (i.e., a=99%). The corresponding month is denoted by *j*. Finally, w_i denotes the weight of the corresponding month. The weights w_i required for $Y2(\theta)$ and $Y3(\theta)$ are based on the monthly peaks of energy demand in Greece for the year 2010 published by the Hellenic transmission system operator (2010). Weights w_i arise from the standardization of that data (Table 1).

Table 1 Monthly energy peak demand of Greece, 2010 (Hellenic transmission system operator, 2010)

Month	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sept	Oct	Nov	Dec
Peak energy demand (MW) Standardized weight (<i>w</i> _j)												

The synthetic time-series generated via stochastic simulation were used as forcing inputs to the simulation model (WEAP21) to drive the simulation (step 4) during the optimization process (step 5). Although, when the simulation model is driven by long synthetic time-series requires long simulation times. For example a single simulation run of WEAP21 driven by 500 years of synthetic data on a 3.0 GHz Intel Core i5 processor with 4 GB of RAM, running on Windows 8 OS requires ~90 s. A typical MOEA requires an order of 10,000 function evaluations to adequately approximate the Pareto front. Consequently, the whole simulation-optimization process would last ~10.5 days, which makes it impracticable and unrealistic for real-world applications.

In order to improve the computational efficiency and ensure the practicability of step 5 we employed surrogate modelling techniques within the context of the optimization process. More specifically we used ParEGO (see Section 2.3); which is a multi-objective surrogate based optimization algorithm and is suitable for expensive function (simulation model) optimization. Surrogate models (or meta-models) are mathematical models that can replace a (computationally) expensive model for the purpose of optimization (e.g., Forrester et al. 2008; Razavi et al. 2012b). In our case the expensive model is the water resources management model (WEAP21).

Prior to employing ParEGO within WEAP21-PSO for the development of uncertaintyaware operational rules a preliminary assessment of the algorithms' performance is performed. ParEGO is compared against the well-known multi-objective evolutionary algorithm NSGAII (Deb et al. 2002) using the available historical data. Both NSGAII and ParEGO were implemented in MATLAB. The comparison of the algorithms was held using historical data due to the reduced computational time required by the simulation model (a single WEAP21 simulation driven by historical data required ~10 s.) thus an adequate approximation of the Pareto front was practically possible when using NSGAII that requires many function evaluations.

2.2 Brief Introduction to Surrogate Based Optimization

SBO incorporates surrogate models (SM) within their iterative process to reduce the computational effort required. Within this framework expensive function evaluations are limited to minimum and performed only to improve the accuracy of the results. The basic steps of a typical SBO framework are; the first step is the initial design which is usually performed with a Design of Experiments (DoE) method. The purpose of DoE is to maximize the information obtained with limited number of samples. A comprehensive review of DoE methods was presented by Giunta et al. (2003). The second step is the construction of the SM; then the SM is searched (optimized/explored) with an internal optimization algorithm. Finally, the next possible samples are identified and evaluated with the expensive model and the surrogate model is updated to improve its accuracy. The iterative process continues until the termination conditions are satisfied, which in many cases (as in this work) is the number of maximum function evaluations. Typical SM are polynomial models, artificial neural networks (ANN), support vector machines (SVMs), Gaussian processes, Kriging and radial basis functions (RBF). Comprehensive reviews of the available methods are available in literature (Forrester et al. (2008); Jin (2011); Kleijnen (2009); Knowles and Nakayama (2008)). Additionally, Razavi et al. (2012a) recently presented a numerical assessment of SBO approach in computationally intensive applications within the context of water resources.

2.3 The ParEGO Algorithm

ParEGO (derived from: Pareto-EGO) is a global optimization algorithm suitable for timeexpensive multi-objective optimization problems (Knowles 2005). ParEGO is essentially a multi-objective extension of Efficient Global Optimization algorithm (EGO, Jones et al. 1998) that making use of scalarizing weight vectors at each iteration in order to gradually approximate the Pareto front. ParEGO algorithm is based on the design and analysis of computer experiments (DACE⁴) model (Sacks et al. 1989) and employs Kriging (Krige 1951) as surrogate model. ParEGO uses Kriging (Ordinary Kriging in our case) to fit previously evaluated points, and using this to estimate interesting new points to visit subsequently. One of the advantages of Kriging (which is used in both EGO and ParEGO) is that a confidence interval of prediction is available and used to guide the search. The iterative process of ParEGO is shown in the flow chart of Fig. 1. Briefly An initial set of solutions are generated using the Latin hypercube (Giunta et al. 2003; Press et al. 1992) and evaluated with the expensive function (or simulation model; WEAP21), the objectives are aggregated into singleobjective formulation using the Tchebycheff function (Eq. 4), the initial DACE model is fitted to these solutions. Then the algorithm tries to locate a trial solution which is most likely to improve the best fitness found so far. In order to do so an internal optimization algorithm (in this case a typical genetic algorithm (GA, Goldberg 1989) implemented in MATLAB⁵) is used in order to search the surrogate model and find the solution that maximizes Expected Improvement (Eq. 7). Then the solution is evaluated with the real cost expensive function (or simulation model) and the surrogate model (Kriging) is updated (re-build) and the next iteration starts. The iterative process continues until the termination condition is satisfied, which is the number of maximum number of allowed function evaluations.

As mentioned earlier, ParEGO in order to solve multi-objective problems uses the nonlinear Tchebycheff function (Eq. 4) in order to aggregate the objectives into single-objective formulation Knowles (2005). This way Tchebycheff function updates the weighting between the objectives in order to gradually build the whole Pareto front. The Tchebycheff aggregation function is briefly described below:

$$f = \max_{j=1}^{n} \lambda_j f_j + \rho \sum_{j=1}^{n} \lambda_j f_j$$
(4)

where, *fj and* λj (*j*=1,2,..,*n*) are the *j*th normalized objective value with respect to the known (or estimated) limits of the cost space, so that each cost function lies in the range [0,1] and its weight, and ρ is a small positive parameter equal to 0.05 according to Knowles (2005). In order to gradually built the whole Pareto front a weight vector is drawn uniformly at random from the set of evenly distributed vectors defined by,

$$\Lambda = \left\{ (\lambda_1, \lambda_2, \dots, \lambda_n) \middle| \sum_{j=1}^n \lambda_j = 1, \lambda_j = \frac{l}{S}, l \in \{0, \dots, s\} \right\}$$
(5)

With $|\Lambda| = (s + k - 1 k - 1)$, so the choice of s determines how many weight vectors there are in total.

⁴ A MATLAB toolbox is available by Lophaven et al. (2002).

⁵ MATLAB Global Optimization Toolbox



Fig. 1 ParEGO algorithm flowchart

As far it concerns the Kriging model it is consisted by two terms the approximated response is expressed as:

$$\hat{y}(\mathbf{x}) = f(\mathbf{x}) + z(\mathbf{x}) \tag{6}$$

The first term is a regression function $f(\mathbf{x})$ and the second is a centered Gaussian process $Z(\mathbf{x})$ with zero mean and variance σ^2 . As suggested by Jones et al. (1998) when there is no prior knowledge of the trend function (as in our case) it is preferably to use constant $f(\mathbf{x})$. This version of Kriging is known as Ordinary Kriging (OK). Details about the mathematical background of Kriging model can be found in literature (Forrester et al. 2008). When dealing with OK, Eq. (6) can be viewed as random field with (unknown) mean β . The second term $Z(\mathbf{x})$ is defined by the covariance which is given by $Cov(Z) = \sigma^2 \Psi(\mathbf{x}^i, \mathbf{x}^j)$ where, $\Psi(\mathbf{x}^i, \mathbf{x}^j)$ is an $n \ge n$ correlation matrix. The elements of that matrix are given by the correlation function $\Psi(\mathbf{x}^i, \mathbf{x}^j) = \exp[-d(\mathbf{x}^i, \mathbf{x}^j)]$ where, $d(\mathbf{x}^i, \mathbf{x}^j) = \sum_{m=1}^k \theta_m [|\mathbf{x}_m^i, \mathbf{x}_m^j|^p]$, *i* and *j* denote the training points, *m* the design parameter, *k* is the number of total design parameters, θ and *p*, are the hyperparameters of correlation function. Parameter *p* determines the initial drop in correlation as distance increases. Lower values of *p* are more suitable for a rougher response surface as they permit a more significant variance in function values for closer points. Parameter θ (or "width"), demonstrates how far a sample point's impact extends (Forrester et al. 2008). In this

work the generalized exponential correlation function is used $(0 \le p \le 2)$. Finally the correlation

function hyperparameters θ and p, are identified by using the Maximum Likelihood Estimation (MLE) method to ensure the best fit (Forrester et al. 2008; Sacks et al. 1989). After the surrogate model is build the next step (see Section 2.2 and Fig. 1) is to search/optimize it using an infill criterion, which in this is Expected Improvement (EI). The evaluation of EI is based on the following equation:

$$EI(\mathbf{x}) = (y_{\min} - \hat{y}(\mathbf{x}))\Phi\left(\frac{y_{\min} - \hat{y}(\mathbf{x})}{\hat{s}(\mathbf{x})}\right) + \hat{s}(\mathbf{x})\varphi\left(\frac{y_{\min} - \hat{y}(\mathbf{x})}{\hat{s}(\mathbf{x})}\right) \qquad if \ \hat{s}(\mathbf{x}) > 0 \qquad (7)$$

$$0 \qquad if \ \hat{s}(\mathbf{x}) = 0$$

where, $\Phi(\cdot)$, $\varphi(\cdot)$ and $\hat{s}(\mathbf{x})$ denote the cumulative distribution function, probability density function and Kriging error respectively.

3 Study Area: The Nestos Hydrosystem

3.1 General Description

The Nestos basin is a trans-boundary basin which extends between Bulgaria and Greece. Nestos Fig. 2a is the second larger river of Thrace water district and one of major rivers in Greece. It flows from Mount Rila in Bulgaria (a region with the highest altitude of the Balkans, about 2.925 m) and has a total length of 234 km of which 130 are in Greek territory. Nestos flows into Greece from the plateau of Nevrokopi of Drama. The bed of the river forms a natural boundary between Bulgaria and Greece for a few kilometers. The Nestos basin is 6.219 km² and about 60 % belongs to Bulgaria. The Greek part of the basin occupies an area equal to 2.525 km² (Paraskevopoulos – Pangaea 1994). The river flows into the Sea of Thrace opposite of Thasos, forming a large delta area about 50 km². It is worth noting that the Nestos estuary is an area protected by the Ramsar Convention and has joined the network NATURA 2000. The first dam built in the region was the dam of Toxotes (1960–1966). This is an irrigation dam with length of 280 m located in the neck of the estuary and diverts the quantities of water to the east (Xanthi) and west (Kavala) bank of the main stream of the river. The first feasibility study of the Toxotes dam was undertaken in 1954 (YDE 1954). Later (1971–1972) a feasibility study for the construction of three more dams upstream was also undertaken. The project began 10 years later (mid-1980s) based on an interim agreement with Bulgaria on minimum incoming water quantities in Greece. In 1995 an agreement was signed for Bulgaria to allow at least 29 % of the total river flow to reach Greece. The original plan was to build three hydropower reservoirs (serially) the first two reversible. These reservoirs were Thysavros (381 MW), Platanovryssi (116 MW) and the Temenos reservoir (19 MW). These projects are multi-purpose projects to provide water for irrigation, distribute water to small towns and industrial areas, and energy production. Thysavros reservoir is largest and the head and of the group project and thus provides scaling and setting of annual runoff of the river. However the overall project has not completed yet due to lack of funds, till now two reservoirs have been constructed: the reservoirs of Thysavros (1996-1997) and Platanovryssi (1998-1999). The third reservoir, Temenos, remains unconstructed but recent developments regarding the privatization of public infrastructures revived interest in its completion. One of scopes of this study is investigates its significance within the context of the full hydrosystem.



Fig. 2 a Geographical representation of the river basin Mesta/Nestos (Skoulikaris et al. 2008). **b** Full hydrosystem modelled in WEAP21 and detail (inside the circle) of simulation of pump-storage. Symbol (\bigcirc) represents the catchments, (\bigcirc) represents the demand nodes, (\bigotimes) represents in-stream flow requirements, (\rightarrow) represents the river, (\bigcirc) represents river nodes or junctions and (\triangle) represents the reservoirs

3.2 Modelling the Hydrosystem of Nestos

The hydrosystem was modeled using WEAP21 simulation model (Fig. 2b). Data from hydrometeorological stations were used to calibrate the rainfall-runoff module within WEAP21. Key inputs for WEAP21 model were: Time-step and time horizon of simulation; reservoirs' properties; inflow from Mesta basin (Bulgarian basin); time-series of precipitation, evapotranspiration and measured flow; water and land uses properties. Due to lack of data the model was calibrated for the period 1/1/1968-31/12/1982 using a monthly time-step. Rainfall data were used from 8 nearby stations and due to lack of data, evapotranspiration from Thessaloniki station was used corrected by a coefficient (1.414) (Skoulikaris et al. 2008).

The rainfall data were spatially distributed using Thiessen polygons and then entered in WEAP21 sub-catchments. As inflow from the upstream Mesta basin the observed flow of Momina Kula station (in Bulgaria) was used. The decision variables used in calibration were the effective precipitation (*Effp*) of the entire catchment for the odd months (Jan, Mar, May, Jul, Sep, Nov); the interim values were calculated with linear interpolation. So the total decision variables were 6. The calibration of the model was performed using the simulated annealing algorithm (Černý 1985; Kirkpatrick et al. 1983) with observed flow at Temenos station (which is the same position with Temenos reservoir, shown in Fig. 2b). The performance measure was Nash-Sutcliffe efficiency (NSE; Nash and Sutcliffe 1970). The NSE value

obtained was 0.875 (after 4000 iterations), which could be considered satisfactory. The optimum decision variables were for Jan=21.32 %, Mar=3.21 %, May=35.93 %, Jul= 82.06 %, Sept=88.82 % and Nov=77.80 %. It is worth mentioning that the low *Effp* value (thus higher direct runoff) of March is probably attributed to the lagged snowmelt process at the Bulgarian part of the basin. The results of calibration were validated for the period 1/1/1991 - 1/12/1994. The obtained NSE for the validation was 0.6945, which is also considered satisfactory. Subsequently, the reservoirs were introduced to the model to simulate the hydrosystem. WEAP21 doesn't have a built-in module to simulate the pump-storage process; hence the process was simulated with the use "dummy" demand nodes (D1 and D2) with the appropriate connectivity (Fig. 2b).

In order to define the maximum monthly turbine/pump discharge of the reservoirs it was assumed that the reservoirs operate 18 h a day as turbines (energy production) and 6 h as pumps (consumption). This assumption was considered reasonable and representative of the current operational rules due to the pump-storage module of the system. Also there is water demand below Toxotes reservoir which irrigates the river Delta (Apr=11.5 m³/s, May= 15.7 m³/s, Jun=18.5 m³/s, Jul=20.9 m³/s, Aug=20.0 m³/s and Sept=13.0 m³/s) and Xanthi future demand node (Apr=5.7 m³/s, May=7.8 m³/s, Jun=9.2 m³/s, Jul=10.4 m³/s, Aug= 10.0 m³/s and Sept=6.5 m³/s). Finally, there is a constant environmental flow requirement equal to 6 m³/s.

Two infrastructure scenarios were investigated, one with the future reservoir of Temenos (scenario 1) and one without it (scenario 2). As far it concerns the preliminary assessment of optimization algorithms, a comparison between NSGAII and ParEGO was performed with the use of historical data (1968–1982) due to lower computational requirements. In this case the employed performance criteria were YI and Y2. As far it concerns the development of uncertainty-aware operational rules within PSO framework the generated synthetic timeseries were based on all available historical data (1968–1982 and 1991–1994) and had length of 500 years. Table 2 summarizes all configurations investigated in this study. It is worth mentioning again that the results based on historical data were used only to compare the two algorithms while the WEAP21-PSO framework uses monthly synthetic time-series to take into account hydrological uncertainty and investigate the responsiveness of different operational policies under different hydrological regimes.

The performance criteria $Y1(\theta)$ and $\Upsilon2(\theta)$ were applied to all configurations and $Y1(\theta)$ and $\Upsilon3(\theta)$ applied only for development of uncertainty-aware operational rules with PSO. The desired reliability for hydropower production was set to a=99 % for all configurations. The pair $Y1(\theta)$ and $\Upsilon2(\theta)$ will be referred as set A while $Y1(\theta)$ and $\Upsilon3(\theta)$ as set B.

Purpose	Algorithm comparison	Development of uncertainty-aware operational rules with WEAP21-PSO
Simulation period Scenario 1 (with Temenos res.) Scenario 2 (without Temenos res.)	Historical time-series (15-years) NSGAII and ParEGO	Synthetic time-series (500-years) ParEGO
Optimization objectives	$YI(\theta)$ and $\Upsilon 2(\theta)$ (Set A)	$YI(\theta)$ and $\Upsilon 2(\theta)$ (Set A) $YI(\theta)$ and $\Upsilon 3(\theta)$ (Set B)

Table 2 Summary of configurations examined in this study

4 Results and Discussion

4.1 Preliminary Assessment of Optimization Algorithms Based on Historical Data

In order to assess the effectiveness of ParEGO, a comparison with NSGAII was held. ParEGO algorithm was run for 150 and 300 function evaluations (FE), while NSGAII for 10,000 FE. The comparison was based on historical data (1968–1982) while both scenarios 1 and 2 were examined. The objective functions used in both cases were Y1 and Y2 (set A). As shown Fig. 3a and c, ParEGO is able to provide a good approximation of the Pareto front for both scenarios (compared to NSGAII). Additionally, it shown that increasing the number of FE to 300 (from 150) the attained surface is slightly better concerning scenario 1 and significant better when comparing scenario 2. Furthermore, this preliminary assessment provides an early insight of the contribution of Temenos reservoir in increasing the hydropower capabilities of the hydrosystem. In order to depict the different operational rules expressed through the objectives trade-off two solutions (upper and lower) from each scenario are selected to investigate in depth. As it was anticipated and shown in Fig. 3b and d, solutions U1 and U2 achieve higher values of mean monthly energy during the summer months, which is critical in order to be able to cover the excessive energy demand of that period. Although, note that this energy is not guaranteed for a certain reliability level and it's just an average expectation. Solutions L1 and L2 seems to balance the monthly temporal distribution of energy and thus are able to produce more firm energy for the desired reliability level (a=99 %). It is worth mentioning that the contribution of Temenos reservoir is notable in both increasing the mean monthly energy and as well as the firm energy. On the other hand it is important to note that



Fig. 3 Attainment surface for NSGAII and ParEGO for scenarios 1 (a) and 2 (c), using historical data of 15 years and energy-duration curves and mean monthly energy for selected solutions (b) and (d) for scenarios 1 and 2 respectively

derivation of operational rules solely based on historical data ignores hydrological uncertainty (and climatic variability) thus it is not suitable for safely inference about the hydrosystems' performance.

4.2 Development of Uncertainty-Aware Operational Rules with WEAP21-PSO

As mentioned above the use of stochastic simulation (thus using synthetic time-series as forcing input to the model) is a technique to take into account uncertainties related with the future inflows of the reservoirs; in order to incorporate these uncertainties and assess the responsiveness of different operational policies, optimization was held using synthetic time-series as forcing input. In this case scenarios 1 and 2 were optimized under two different sets of objectives (set A and B) (see Section 2.1). Figure 4a and c presents the Pareto fronts of scenario 1 and 2 for both optimization objective sets. In order to depict some energy related properties of hydrosystem the energy-duration curves (EDC) of Fig. 5b and d are constructed for two solutions (the upper and the lower, denoted by U and L respectively) for each configuration. EDCs demonstrate the monthly energy produced from the hydropower reservoirs for a certain percentage of time, i.e., for a certain reliability level. The constructed trade-offs and EDCs demonstrate the significance of Temenos reservoir, which contributes to the increase of, guaranteed (99 % reliability level) constant firm energy approximately by 20 GWh (\approx +22 %).

As far it concerns objective set A, it provide a wide trade-off with a variety of possible operational rules. For scenario 1 the firm energy varies between 55.7 and 71.9 GWh, while for scenario 2 between 38.9 and 52.7 GWh. Additionally when comparing scenario 1 and 2, the



Fig. 4 Pareto fronts of scenarios 1 and 2 for objective sets A (a) and B (c). Energy-duration curves for selected solutions of scenarios 1 and 2 for objective sets A (b) and B (d)



Fig. 5 Energy related properties for selected solutions of scenarios 1 and 2 for objective sets A (a, b) and B (c, d)

weighted sum of average monthly energy is increased by 240-320 units. This criterion weights (according to peak energy demand in Greece) the temporal variation of the mean monthly energy; the monthly variation is illustrated clearly for selected solutions in Fig. 5a and b.

As far it concerns objective set B, it is worth noting that the energy-duration curves are almost identical for the upper and lower solution for each scenario; 71.9–72.6 GWh for scenario 1 and 50.4–52.7 GWh for scenario 2. The reason is that both objectives of set B are related with firm energy (YI). Although, objective Y3 weights the temporal variation of monthly firm energy in order to line firm energy generation with peak energy demand.

Figure 5 depicts the temporal variation of average monthly energy for both scenarios and both objective sets, additionally distinct the produced energy to firm and secondary. As far it concerns objective set A, the annual firm energy varies from 867 to 911 GWh for scenario 1 and from 670 to 687 GWh for scenario 2. A slightly different behavior (due to the nature of objective function *Y3*) is observed for objective set B, where the annual firm energy varies in smaller range; from 925 to 936 GWh for scenario 1 and from 706 to 717 GWh for scenario 2. In this configuration the solutions provide more stable temporal distribution of energy during the year and high peaks during the summer months. From the distinction of energy to firm and secondary we can infer that Temenos reservoir significantly contributes to the increase of firm energy (~200 GWh), thus extends the hydrosystems' energy base, i.e., the system can produce more than ~200 GWh annually without compromising energy reliability. Furthermore, the use of criteria *Y2* and *Y3* indicate that a small loss in the monthly firm energy can lead to an increase of monthly specific firm energy. This way higher firm energy can produced during months that present major energy demand peaks.

Table 3 summarizes the energy related properties for each reservoir separately concerning the selected solutions. From the table below can be perceived that the presence of Temenos

Reservoir	Thysavros		Platanovryssi		Temenos				
Property/ Solution	Average monthly energy (GWh)	Firm energy (GWh)	Average monthly energy (GWh)	Firm energy (GWh)	Average monthly energy (GWh)	Firm energy (GWh)			
Objectives: set A									
U1	66.4	47.0	28.9	20.7	5.1	2.3			
L1	67.2	39.6	29.0	14.8	5.2	0.4			
U2	66.5	43.4	15.3	8.7	_	-			
L2	67.1	37.7	15.3	1.2	_	-			
Objectives: set B									
U1	66.6	49.4	29.0	20.0	5.2	2.4			
L1	66.8	48.3	29.0	19.9	5.2	2.3			
U2	66.5	43.6	15.3	8.8	_	-			
L2	66.6	42.4	15.3	7.5	-	_			

 Table 3
 Reservoir specific energy related properties for selected solutions of scenarios 1 and 2 for objective sets

 A and B

contributes also to the comprehensive operation of Platanovryssi reservoir. It is evident that besides Temenos own contribution to the total produced energy, the main benefit derives from the capability of reservoirs (Platanovryssi-Temenos) to operate in pump-storage mode. In scenario 2, Platanovryssi reservoir almost doubles its (energy) contribution to the hydrosystem.

Finally, it is worth noting that all scenarios and configurations explored in this study were able to satisfy irrigation water demand and environmental requirement with 99-100 % reliability. This is attributed to the high water inflows of the reservoirs and due to the fact that irrigation water demand and environmental flow requirement are relatively small, and do not exceed the total of 100 million m³ in any time-step.

5 Conclusions

This paper employs long synthetically generated (through stochastic simulation) time-series within multi-objective Parameterization-Simulation-Optimization (PSO) framework to develop uncertainty-aware operational rules for the challenging, trans-boundary hydrosystem of Nestos. Furthermore, infrastructure scenarios concerning the construction of a future reservoir (Temenos) are explored. The results demonstrate that the reservoir of Temenos contributes significantly to the increase of monthly firm energy production (\approx +22 %) and additionally it can be deduced that the reservoir not only contributes to energy production but ensures the fully and smooth operation of the full hydrosystem. The major energy benefit from the construction of Temenos arises from the comprehensive operation of pump-storage mode with the upstream reservoir (Platanovryssi). Furthermore, the optimization criteria (two of them were focused on the temporal variability of monthly energy generation) used in this study provided robust results and useful insights related with hydropower energy production with high reliability. Additionally, the operational rules derived in this study were able (for all scenarios) to provide 100 %coverage of irrigation water demand and environmental flow requirement. As far it concerns the practicability of the method, the computational overhead that stems from the use of long synthetic time-series was confronted with the use of surrogate based optimization techniques within PSO framework. More specifically we employed ParEGO, which proves to be a fast and effective method (compared to NSGAII) in deriving robust uncertainty-aware optimal operational rules within few model simulations (~150–300). The algorithm is particular useful when the objective functions are expensive (in terms of simulation time) to evaluate or when there is a computational (or time) budget limitation. Summarizing the coupling of WEAP21 with MATLAB and the use of surrogate based optimization (SBO) algorithms extends the capabilities of the simulation model (WEAP21-PSO) and leads to optimal, robust and uncertainty-aware solutions; this way problems related with water-energy management can be effectively and practicably confronted within reasonable computational time.

Acknowledgments This research was undertaken within the project "Investigation of climate change in Greece and its impact on the sustainability of projects dealing with hydroelectric power and the agricultural economy: Application in the Nestos river basin d KLIMENESTOS" which was financed by the Greek Ministry of Education, Lifelong Learning and Religious Affairs, General Secretariat for Research and Technology, through the National Strategic Reference Framework (NSRF) 2007–2013 and under the operational programmes "Competitiveness and Entrepreneurship and Regions in Transition", within the National Action "Cooperation 2009".

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