1. Abstract
We investigate the computational challenges of a model for the integrated simulation—optimization of water and renewable energy fluxes, based on an example (hypothetical) hybrid water—energy system at a small non-connected island (Astypalaea, Greece). The system consists of a hydroturbine reservoir with pumped storage facilities, connected with systems of wind and solar power plants. The model runs on hourly time step, using as inputs rainfall and temperature data, data for the water supply, irrigation and electric energy demands, as well as energy production data from wind and solar resources. The reservoir system attempts to fulfill the two water demands and regulate the energy excesses and deficits. Due to the fine time step of calculations and the use of synthetic time series of long horizon, the computational burden of simulation runs in an optimization framework is significant. In an attempt to minimize the computational load, particularly in optimizations, we investigated the use of surrogate approaches, through black-box sub-models (e.g., neural networks) that represent autonomous parts of the whole simulation procedure. The outcomes of surrogate models are compared with the corresponding outputs of the original model.

2. Study area and data
- Astypalaea (Astrotókia) is a Greek island with 1334 residents (2011 census), that belongs to the Dodecanese complex (total area 97 km²).
- Livadi reservoir, which fulfills domestic, touristic and agricultural uses, is considered element of a hypothetical hybrid renewable energy system.
- Key characteristics (actual or estimated):
  - Catchment area 8.0 km²
  - Net capacity 875 000 m³
  - Surface at max elevation 105 000 m²
  - Mean inflows 700 000 m³/day
  - Water supply demand 210 000 m³/y
  - Agricultural demand 230 000 m³/y
  - Total energy demand 6250 MWh/y
  - Water-energy components (hypothetical):
    - Hydropower plant, installed at the discharge outlet (max head 32 m, discharge capacity 1000 m³/h, efficiency 0.85)
    - Pumped storage tank, for regulating hourly energy deficits and surpluses (tank capacity 50 000 m³, max head 200 m, discharge capacity 1500 m³/h, efficiency 0.85 and 0.80, in the two directions).
    - Solar and wind plants of 0.5 MW each, with estimated energy production 162 and 116 MWh/y, respectively.

3. The challenging water-energy modelling problem
The modelling challenge:
- The representation of two simultaneous fluxes (water & energy) and their interactions increases the number of variables and constraints, as well as the conflicts of decisions.
- Since energy production from renewables (hydropower, solar, wind) is driven by randomly varying meteorological processes, stochastic approaches are essential to provide synthetic input data of large length and fine temporal resolution (at least hourly).

Major computational issues to handle:
- Increase of simulation burden, due to the significantly larger complexity of the process representation problem;
- Substantial increase of simulation steps, due to the use of hourly synthetic data of long time horizon (in contrast to monthly steps that are typically employed in typical water management problems);
- Need to run in optimization mode, also considering more control (or design) variables than in typical hydrosystem models.

4. Detailed simulation models for hydrological and energy fluxes and their surrogates

4.1. Hydrological and water demand simulation model
- Daily time step;
- Meteorological drivers: rainfall, temperature;
- Modelling components:
  - Parametric rainfall-runoff model, with three parameters: runoff & actual evapotranspiration (PET, P);
  - Irrigation model: agricultural water demand (fPET, fATT);
- Water supply model (drinking water demand & temperature)

Reservoir operation model
- Hourly time step;
- Model inputs:
  - Daily runoff, evaporation, water demands (outputs of hydrological model, disaggregated from daily to hourly resolution);
  - Energy deficit and excess (outputs of energy balance across the island);
- Model outputs:
  - Water abstractions for water supply and irrigation;
  - Energy production and consumption through the energy components;
- Key assumptions:
  - Abstractions from the intake are only made for providing drinking and agricultural water, not for producing energy (thus, the power plant downstream of the intake is not driven by the energy deficits);
  - The regulation of energy deficits or surpluses are employed through the pumped-storage system;
  - The water storage at the upstream tank can be also used for fulfilling drinking water demand, in case of limited storage at the main reservoir;
  - In case of water excess, we first attempt to pump water to the upstream tank (to minimize water losses), next release from the intake (to take advantage of energy production), and finally release through the spillway.

4.2. Hydrological and water demand simulation model

5. Detailed simulation models
Hydrological and water demand simulation model
- Daily time step;
- Meteorological drivers: rainfall, temperature;
- Modelling components:
  - Parametric rainfall-runoff model, with three parameters: runoff & actual evapotranspiration (PET, P);
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5. Detailed simulation models

6. Surrogate models
General setting of surrogate approaches
- Artificial neural networks (ANNs) with one hidden layer;
- Training with historical data, via Bayesian regularization backpropagation;
- Data breakdown: 70% training, 15% validation, 15% test;
- Hydrological simulation model
  - Investigation of different structures, by changing the inputs, the number of neurons and the outputs;
  - The simplest structure used two distinct ANNs with common inputs (rainfall & temperature of current day), to provide the runoff and actual ET, respectively;
  - More complicated structures also used antecedent rainfall data, for time lags from one to 50 days;
  - Dynamic structures (nonlinear autoregressive) were also examined, to account for storage effects that are of major importance in all hydrological processes;
  - Although even the simplest structures ensured good efficiency in training (93% for runoff and 85% for actual ET), they performed worse when the tests were stressed against synthetic data of 100 years length.

Reservoir operation model
- Two approaches were examined, using the actual hydrological inputs and the estimations provided by the surrogate hydrological model.
- Both were driven with the two water demand time series and the energy deficit and excess data, at the hourly scale.
- Since our emphasis is to energy, we only considered one output, i.e., the energy deficit and excess after employing water abstractions and regulations.
- Although the two approaches ensured same efficiency in training with historical data (79%), we preferred the structure driven with actual hydrological data, since this ensured better efficiency when fed with synthetic inputs.

In stochastic simulation mode, i.e., using 100 years of synthetic hourly inputs, the detailed model ran in 175 seconds, while the surrogate model in only 3 seconds (all computations have been automated in MATLAB environment).

7. Comparison of model outputs

8. Conclusions
- At present, renewables have an integral role in energy planning and management at all spatial scales (national, peripheral, local), also revealing the key importance of water both as energy producer and regulator.
- Stochastic simulation approaches that have been successfully employed in water resources planning and management, are essential for representing the complexities and uncertainties of conjunctive water and energy systems, especially in computational burdens.
- Surrogate approaches through ANNs is a promising solution towards ensuring substantial reduction of the computational effort of this problem, thus revealing a new challenge for the hydrological community.
- Preliminary analyses in this hypothetical study were encouraging, however more structures and training approaches have to be tested to improve the structural efficiency of ANNs in stochastic mode.
- Actually, the great challenge is providing surrogate schemes that are stressed against synthetic data, which allows investigating their behavior under a wide spectrum of feasible conditions.

References