

European Geosciences Union General Assembly 2012 Vienna, Austria, 22-27 April 2012

Session HS5.5

Models and computational methods for management and optimization of controlled water resources systems

A Monte Carlo approach to water management



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Presentation available online: itia.ntua.gr/1199/

What do we really mean by management/control?

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Can management rely on deterministic future predictions?





General characteristics of water management problems

- Hydrosystems are nonlinear with respect to their dynamics, operation constraints and objectives
 - Linear programming methods are extremely effective but are inappropriate except for simple sub-problems within water management
- Water management problems cannot be divided into sequential stages
 - The overall reliability and performance cannot be assessed unless a global view is acquired; thus, dynamic programming methods are inappropriate
- Water control problems may involve many variables
 - However, a parsimonious representation, in which the number of control variables is kept at a minimum has advantages
- Typical problems are highly nonconvex in terms of objective functions and constraints, so that numerous local optima appear very often
 - This renders classical (deterministic) optimization methods useless
- Uncertainty is always present, albeit often missed to include in modelling
 - Deterministic methods cannot deal with the uncertainty of future conditions (inflows, demands, etc.); even stochastic extensions of these methods (e.g. linear-quadratic-Gaussian control) necessitate drastic oversimplifications that make the obtained results irrelevant to reality
- Problems may be **multiobjective** (may involve several performance criteria)

What is the Monte Carlo method?

- Is it a method to generate random numbers?
- Is it a method to perform random computer experiments?
- Is it a method to deal with problems that involve randomness?
- Is it a method to fool people when proper mathematical methods become too difficult?
- Definition (adapted from Wikipedia): The Monte Carlo method is a class of computational algorithms that rely on repeated random sampling to compute their results
- Note: "Monte Carlo" is synonymous to "stochastic"
- In other words, the Monte Carlo method is a numerical method which, like other numerical methods, becomes useful when analytical solutions do not exit (that is, almost always...)
- While the Monte Carlo method seems to be a natural choice when the problem studied involves randomness, it is also powerful even for purely deterministic problems

Stanislaw Ulam, the solitaire and the conception of the Monte Carlo method

STAN ULAM, JOHN VON NEUMANN, and the MONTE CARLO METHOD

The Monte Carlo method is a statistical sampling technique that over the years has been applied successfully to a vast number of scientific problems. Although the computer codes that implement Monte Carlo have grown ever more sophisticated, the essence of the method is captured in some unpublished remarks Stan made in 1983 about solitaire.

"The first thoughts and attempts I made to practice [the Monte Carlo method] were suggested by a question which occurred to me in 1946 as I was convalescing from an illness and playing solitaires. The question was what are the chances that a Canfield solitaire laid out with 52 cards will come out successfully? After spending a lot of time trying to estimate them by pure combinatorial calculations, I wondered whether a more practical method than "abstract thinking" might not be to lay it out say one hundred times and simply observe and count the number of successful plays. This was already possible to envisage with the beginning of the new era of fast computers, and I immediately thought of problems of neutron diffusion and other questions of mathematical physics, and more generally how to change processes described by certain differential equations into an equivalent form interpretable as a succession of random operations. Later...[in 1946, 1] described the idea to John von Neumann and we began to plan actual calculations."

Von Neumann was intrigued. Statistical sampling was already well known

by Roger Eckhardt

in mathematics, but he was taken by the idea of doing such sampling using the newly developed electronic computing techniques. The approach seemed especially suitable for exploring the behavior of neutron chain reactions in fission devices. In particular, neutron multiplication rates could be estimated and used to predict the explosive behavior of the various fission weapons then being designed.

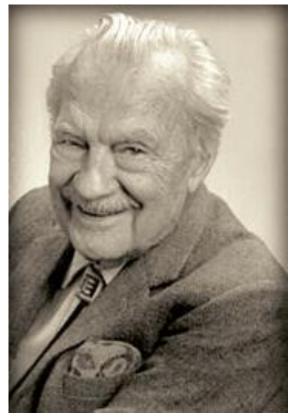
In March of 1947, he wrote to Robert Richtmyer, at that time the Theoretical Division Leader at Los Alamos (Fig. 1). He had concluded that "the statistical approach is very well suited to a digital treatment," and he outlined in some detail how this method could be used to solve neutron diffusion and multiplication problems in fission devices for the case "of 'inert' criticality" (that is, approximated as momentarily static config-



Stanislaw Ulam (13 April 1909 – 13 May 1984): Polish-American mathematician; since 1943 he worked in Los Alamos National Laboratory (Manhattan Project under leadership of Robert Oppenheimer)

Source: Eckhardt (1989)

Nicholas Metropolis and the "birth certificate" of the Monte Carlo method



Nicholas Metropolis (11 June 1915 – 17 October 1999): Greek-American physicist; since April 1943 he worked in the Manhattan Project in Los Alamos

JOURNAL OF THE AMERICAN STATISTICAL ASSOCIATION

Number 247

SEPTEMBER 1949

Volume 44

THE MONTE CARLO METHOD

NICHOLAS METROPOLIS AND S. ULAM Los Alamos Laboratory

We shall present here the motivation and a general description of a method dealing with a class of problems in mathematical physics. The method is, essentially, a statistical approach to the study of differential equations, or more generally, of integro-differential equations that occur in various branches of the natural sciences.

ALREADY in the nineteenth century a sharp distinction began to appear between two different mathematical methods of treating physical phenomena. Problems involving only a few particles were studied in classical mechanics, through the study of systems of ordinary differential equations. For the description of systems with very many particles, an entirely different technique was used, namely, the method of statistical mechanics. In this latter approach, one does not concentrate on the individual particles but studies the properties of sets of particles. In pure mathematics an intensive study of the properties of

Integration: Classical numerical method

 In the numerical integration of a function f of a scalar variable u, a definite integral is approximated by the relationship (known as the trapezoidal rule)

$$\int_{0}^{1} f(u) \, du \approx \sum_{n=0}^{m} w_n f\left(\frac{n}{m}\right)$$

where *m* is a positive integer and w_n denotes a weight, equal to 1 / 2m for the endpoints n = 0 and n = m, and equal to 1 / m for all intermediate *n*

Likewise, in the numerical integration of a function of a vector variable of size s in the space I^s := [0, 1]^s, the relationship becomes

$$\iint_{I^s} f(\boldsymbol{u}) \, d\boldsymbol{u} \approx \sum_{n_1=0}^m \dots \sum_{n_s=0}^m w_{n_1} \dots w_{n_s} f\left(\frac{n_1}{m'}, \dots, \frac{n_s}{m}\right)$$

- The computational nodes form a rectangular grid with equidistance 1/m
- Their number is $N = (m + 1)^s$ and the computational error is $O(m^{-2}) = O(N^{-2/s})$
- Consequently, for a specified acceptable error, N increases exponentially with s (curse of dimensionality)

Integration: The Monte Carlo method

In the Monte Carlo integration, the N points for the evaluation of f(u) are taken at random (rather than at the nodes of a grid) and the weight is 1/N, so that (Niederreiter, 1992)

$$\int_{I^s} f(\boldsymbol{u}) \, d\boldsymbol{u} \approx \frac{1}{N} \sum_{n=1}^N f(\boldsymbol{x}_n)$$

where $x_1, ..., x_N$ are independent random points over the space l^s

• For an arbitrary integration space *B* the relationship becomes

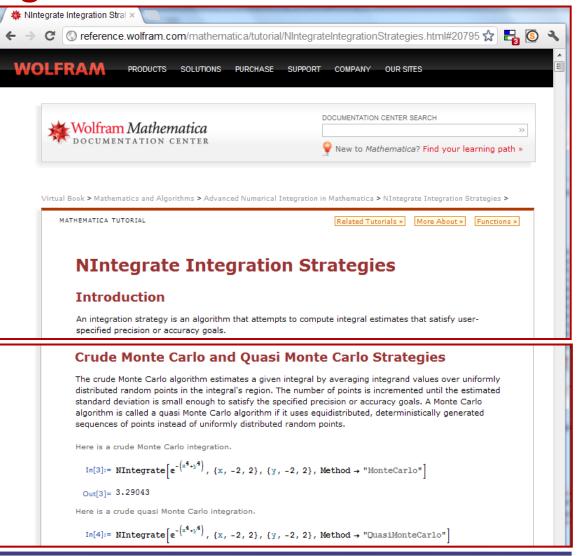
$$\int_{B} f(\boldsymbol{u}) \, d\boldsymbol{u} \approx \frac{1}{N} \sum_{n=1}^{N} f(\boldsymbol{x}_{n}) \, U_{B}(\boldsymbol{x}_{n})$$

where $U_{B}(\mathbf{x}_{n}) = 1$ if $\mathbf{x}_{n} \in B$ while $U_{B}(\mathbf{x}_{n}) = 0$ if $\mathbf{x}_{n} \notin B$; according to a classical statistical law, the computational error is $O(N^{-1/2})$

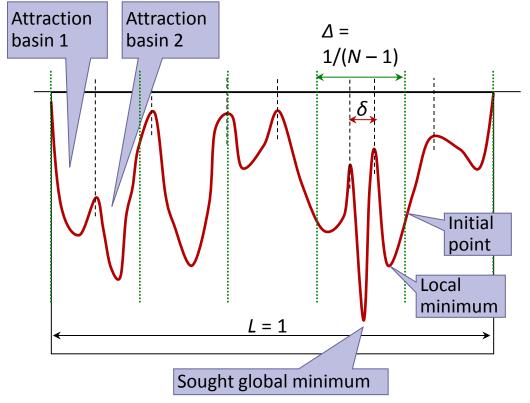
- Observation: The error does not depend on the dimensionality s
- Conclusion: Comparing the errors of the classical and Monte Carlo methods, we readily obtain that the latter is preferable when the dimensionality s > 4
- Remark: For large dimensionality s, e.g. > 20, the classical method is infeasible while the Monte Carlo is always feasible

The Monte Carlo method is part of routine numerical modelling

- The screen on the right shows how the *Mathematica* software implements various versions of the Monte Carlo method for numerical integration
- This is not just an additional option within a repertoire of available options; for high-dimensional spaces it is the only possibility



Typical optimization of a scalar function of a scalar variable: deterministic approach

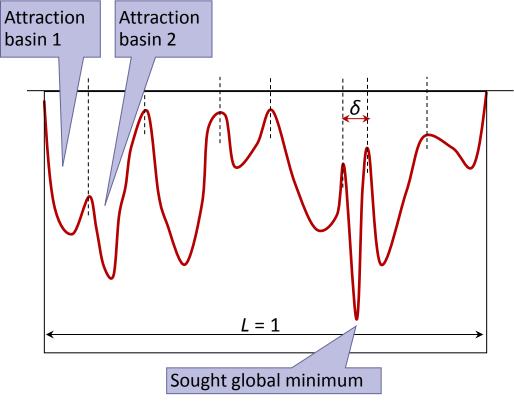


With the chosen $\Delta > \delta$, the global minimum will not be found

- Assumption: We have an effective deterministic local search algorithm (e.g. parabolic interpolation) that, starting from an initial point, will determine the local minimum located in the corresponding attraction basin
- Strategy: We determine the global minimum using a multistart search, starting from a set of N initial points at equidistance ∆ along the axis
- **Conclusion**: We will locate the global minimum if $\Delta \leq \delta$

Hence,
$$N_{\min} \approx 1/\delta$$

Typical optimization of a scalar function of a scalar variable: stochastic (Monte Carlo) approach

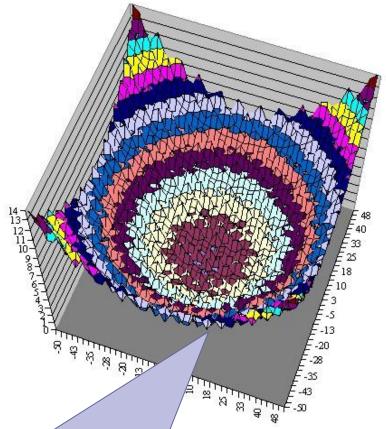


- Assumption: The same as in the deterministic approach
- Strategy: We try a number N of initial points chosen at random
- Conclusion: The probability to locate the minimum with one trial is 1/δ; the probability to find it starting from N initial points chosen at random is

 $p_{\varepsilon} = 1 - (1 - \delta)^{N} \approx 1 - \mathrm{e}^{-\delta N}$

 Hence, even with a few points, there is a possibility (not certainty) to find the minimum

Optimization of a scalar function of a vector variable



An example: the Griewank function for n = 2 $f(x_1, x_2, ..., x_n) = (x_1^2 + x_2^2 + ... + x_n^2)/400$ $-\cos(x_1/\sqrt{1})\cos(x_2/\sqrt{2})...\cos(x_n/\sqrt{n}) + 1$

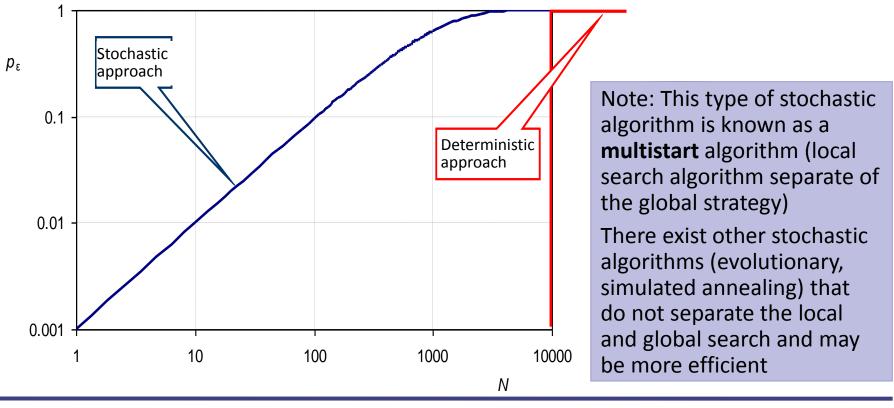
- If the attraction basin at a manifold of dimension *s* (= size of vector variable) has characteristics lengths per dimension $\delta_1, \delta_2, ..., \delta_s$, with volume $\alpha = \delta_1 \delta_2 ... \delta_s$, then:
- According to the deterministic approach (initial points at a grid), the global minimum will be found only if $N_{\min} \approx 1/(\min_i \delta_i)^s$
- According to the Monte Carlo approach, where the initial points are chosen at random, there is always a non-zero probability to find the minimum, equal to $p_{\epsilon} = 1 - (1 - \alpha)^{N} \approx 1 - e^{-\alpha N}$
- Note that δ_i and α are not known a priori

A comparison of the deterministic and stochastic (Monte Carlo) approaches: a numerical example

• We assume a 2D optimization problem with a hypothetical attraction basin $\alpha = \delta_1 \delta_2 = (1/10) (1/100) = 1/1000$

• Deterministic approach: $N_{\min} \approx 1/(1/100)^2 = 10000$

Stochastic (Monte Carlo) approach $p_{\varepsilon} = 1 - (1 - 1/1000)^{N} \approx 1 - e^{-N/1000}$

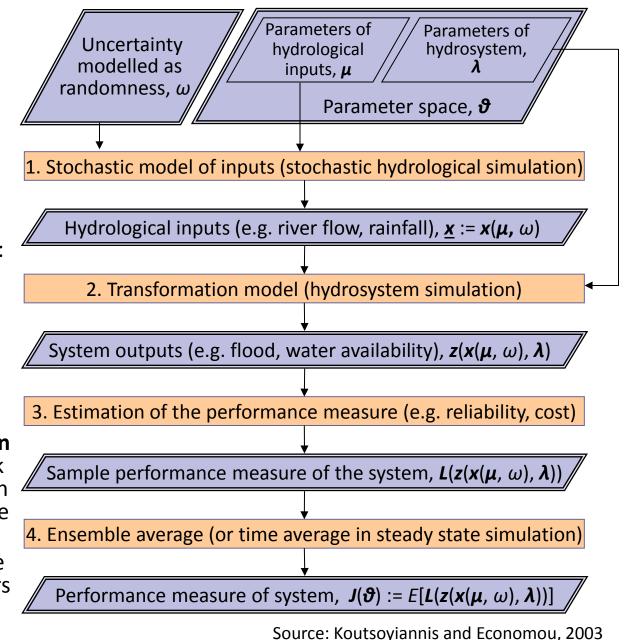


Additional reasons for adopting a stochastic approach in water management

- In water management decisions are made with reference to the future
- The future is (and most probably will always be) unknown
- Methods assuming known future conditions are common but inappropriate
- Only probabilistic approaches offer a scientifically rigorous method to cope with future uncertainty

A general methodological scheme for water management

- Mathematically, water engineering and management problems include two sub-problems:
- An integration problem to find the performance measure of the hydrosystem,
 J(μ, λ) = E[L(z(x(μ, ω), λ))] Note: expectation means integration
- A constrained **optimization** problem, in which we seek the hydrosystem operation parameters λ that optimize the performance $J(\mu, \lambda)$
- For both sub-problems the Monte Carlo method offers a feasible and consistent solution



A demonstration using a simple water management problem: reservoir sizing

"Textbook" methodology (for kindergarten...)

- The problem is stated as follows: If i_t denotes the inflow to a reservoir for time t = 1, 2, ..., n, where n is a control horizon, we wish to find the smallest reservoir storage capacity, λ, that sustains a steady state release d
- Sadly, the textbooks still provide an inconsistent deterministic methodology not differing from the original Ripple (1883) 'mass-curve' technique; although the method is presented as intuitive and helpful for understanding, it develops an incorrect understanding
- Subsequent tabulated versions of the method, e.g. the sequent-peak technique (Thomas and Burden, 1963) are equally misleading
- Other versions of the method that use synthetic, instead of historical, time series (Schultz, 1976) do not make any difference, as long as they do not make consistent use of probability and the notion or reliability
- Reliability, i.e. the probability that the system will perform the required function, was introduced by Hazen (1914)
- Ironically, while Hazen was American, the Americans did not fully embrace the notion of reliability
- It was the Soviet engineering community (Kritskiy and Menkel, 1935, 1940; Savarenskiy, 1940; Pleshkov, 1939) which advanced Hazen's idea
- For a history of the developments on this problem see Klemes (1987)

Linear programming solution (for elementary school...)

There is a linear programming problem formulation (ReVelle, 1999, p. 5), i.e.:

minimize	λ	
s.t.	$s_t = s_{t-1} + i_t - d - w_t$	t = 1, 2,, n
	$s_t \leq \lambda$,	t = 1, 2,, n
	$s_n \ge s_0$	
	$s_t, w_t, \lambda, d \ge 0,$	t = 1, 2,, n

where s_t and w_t is the reservoir storage and spill, respectively, at time t

- While the actual control variable is only one (the reservoir size λ) this formulation uses a number 2*n* of additional control variables, s_t and w_t , as well as a total 3*n* + 3 constraints (e.g. for *n* = 1000, we will have 2001 control variables and 3003 constraints); the high dimensionality is not fortunate
- The tacit assumption is that the future inflows i_t are known
- This formulation assumes full reliability (a = 100%), which is consistent with the deterministic problem formulation; ReVelle (1999) provides another formulation that can deal with reliability a < 100%, but the logical coherence is questionable (why a < 100% if inflows are deterministic?)</p>
- The method can hardly incorporate nonlinear system components (e.g. leakage or evaporation that are nonlinear functions of storage)

Consistent solution (for adults only...)

The consistent formulation is very simple, elegant and generic:

minimize $J(\mu, \lambda) = \lambda$ s.t. $P\{\underline{r}_t = d\} \ge a$ (alternatively $E[\underline{r}_t]/d \ge a$) where λ is the reservoir capacity, μ is a vector of parameters of hydrological inflows, J is the performance measure to be minimized (here equal to λ), $P\{$ denotes probability, a is the acceptable reliability and \underline{r}_t and \underline{s}_t are the reservoir release and storage, respectively, at time t, treated as random variables and deterministically related to inflows \underline{i}_t via the system dynamics, i.e.,

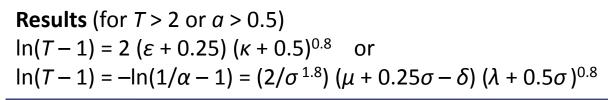
 $\underline{r}_t = \min(d, \underline{s}_{t-1} + \underline{i}_t), \quad \underline{s}_t = \min(\lambda, \max(0, \underline{s}_{t-1} + \underline{i}_t - d))$

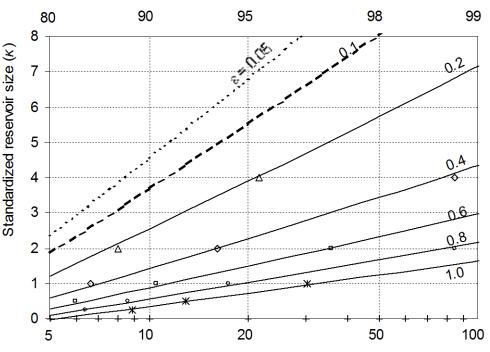
- Here we have only one control variable and one constraint
- The performance measure depends not on the inputs <u>i</u> but on the parameters thereof, μ
- The formulation is highly nonlinear, yet extremely easy to solve (e.g. in a spreadsheet) by Monte Carlo simulation (the integration part refers to the determination of P{<u>r</u>_t = d} or E[<u>r</u>_t])
- Any nonlinear adaptation of dynamics is readily incorporated

Typical results of the consistent method (storage-
yield-reliability relationship)Design reliability level (a, %)

Assumptions and characteristic quantities

- Inflows independent identically and normally distributed (seasonal variation neglected)
- μ : mean inflow
- σ : standard deviation of inflow
- *a* : reliability
- T := 1 / (1 a): return period of reservoir emptying
- d: demand
- λ : reservoir storage capacity
- $\kappa := \lambda / \sigma$: standardized reservoir storage capacity
- $\varepsilon := (\mu \delta)/\sigma$: standardized mean loss

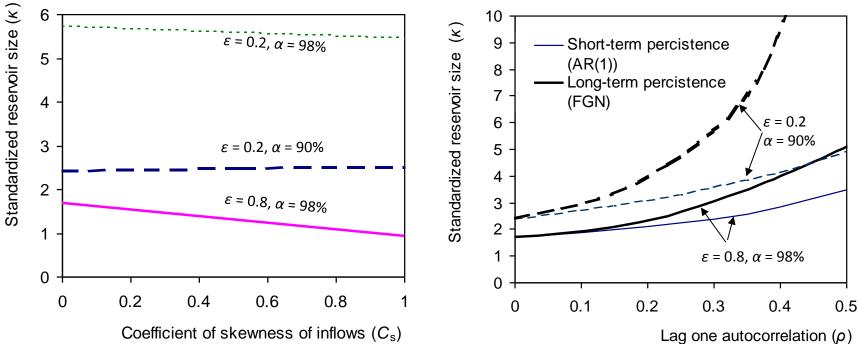




Design return period (T, years)

For details see Koutsoyiannis (2005)

Extensions of results for more complex stochastic structure of inflows



Effect of skewness (Results for independent gamma distributed inflows)

Effect of persistence (Results for normally distributed inflows)

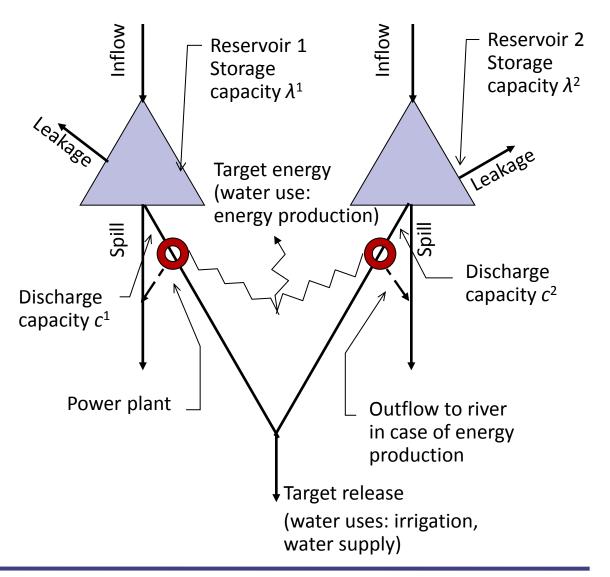
- While the case presented is simple, the method is fully generic and can perform with any type of system dynamics and stochastic structure of inflows
- While there exist in the literature different approaches (e.g. the formulation by Moran, 1954, based on Markov chains, as well as recent attempts) these involve radical simplifications (e.g. discretization of the reservoir space) and their usefulness is questionable
- For details see Koutsoyiannis (2005)

Application to a hypothetical system of two reservoirs

This full study can be found in Koutsoyiannis and Economou (2003)

Hypothetical hydrosystem

- Two reservoirs forming a system that serves a joint objective such as:
- Maximization of release for water supply or irrigation
- Minimization of cost for water conveyance
- Maximization of benefit from energy production



Study details

Tested approach: The general, doubly Monte-Carlo, methodological scheme

Benchmark procedures

- A high-dimensional perfect foresight method (control variables are the complete series of releases) combined with an evolutionary optimization method
- An "equivalent reservoir method", in which the reservoir system is replaced by one hypothetical reservoir with characteristics merging those of the different reservoirs of the system (it provides an upper bound for the system performance for some of the problems)
- Simulation scale: monthly (water supply: 12 months per year; irrigation: 7 months per year)
- Simulation period: 16-50 years, depending on the problem examined, so that the total number of control variables in the high dimensional approach be 400 or less (in order for the problem to be tractable using a typical evolutionary solver)

Parsimonious modelling and the PSO approach

- Referring to a system optimization at a control horizon of 10 years at monthly scale, what is more meaningful result of an optimized system operation e.g. at time step 100 (that is some 8 years from now), for a projected demand of 270 hm³?
 - High dimensional approach (the releases are the control variables): The optimal release from reservoir 1 should be 100 hm³ and that of reservoir 2 should be 170 hm³
 - Parsimonious approach: Determine the optimal releases, not now but then, so that the quantities of water stored in each reservoir have some balance
- The latter approach necessitates the use of an operation rule that quantifies what the *balance* is
- It is reasonable to assume that this quantification should include some parameters, which become the control variables to be determined by the Monte Carlo optimization
- This gives rise to the so-called Parameterization-Simulation-Optimization (PSO) approach

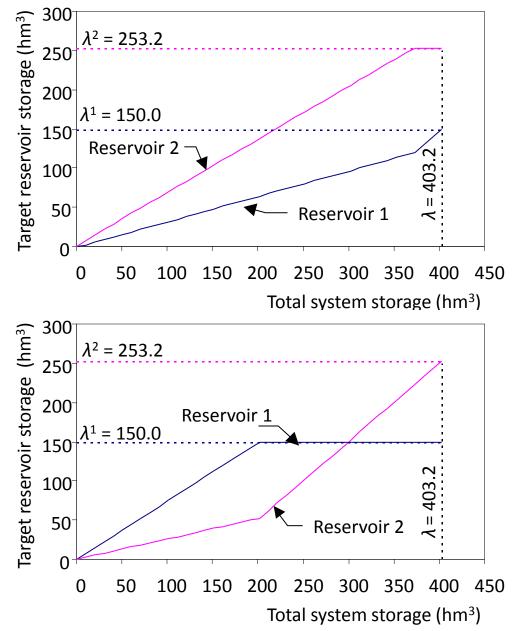
Reservoir system parameterization

A simple operation rule can be formulated so as to give the target storage s^j_{*} of reservoir j as a linear function of the storage capacity of that reservoir, λ^j, and of the system, λ, as well as the total system storage, s, i.e.:

 $s^j{}_* = \lambda^j - \alpha^j \,\lambda + b^j \,s$

where *a^j* and *b^j* are the parameters to be determined (**2 control variables per reservoir**)

- The linear rule needs some nonlinear adjustments to assure physical consistency (Nalbantis and Koutsoyiannis, 1997)
- The figures exemplify the optimized parametric operating rules for one of the examined problems (upper: rule for the refill period; lower: rule for the drawdown period)



Results from a large family of tests

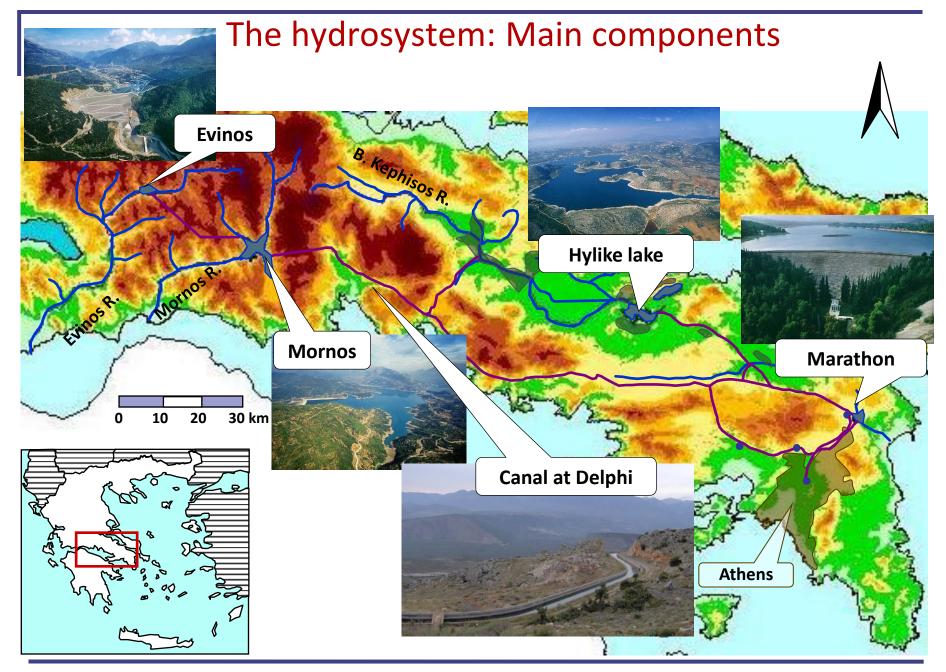
- Maximization of reliable release for water supply or irrigation
 - The PSO methodology with 5 control variables and zero foresight resulted in practically the same performance as in the perfect foresight method with 351 control variables
 - Even with 2 control variables the PSO method with zero foresight is very effective as the reduction in performance is only 1.68%
- Minimization of cost (assuming different unit cost to convey water from each reservoir)
 - The results of the PSO with 4 control variables and zero foresight are almost identical to those of the perfect foresight method with 350 variables (irrigation) or 192 variables (water supply)

Maximization of benefit from energy production

- The reduction in performance of the PSO methodology is no more than 3% with respect to the high dimensional perfect foresight method
- Careful inspection showed that the 3% improvement in the high dimensional method is fake as it is associated with the perfect foresight aspect (avoidance of spill by unjustified more intense energy production in earlier months)
- General conclusion: The PSO method performs practically as well as benchmark methods and has many additional advantages

Application to a demanding real world system: The water resource system of Athens

For details see: Koutsoyiannis and Economou (2003); Koutsoyiannis *et al.* (2002, 2003); Efstratiadis *et al.* (2004)



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Typical problems to be answered

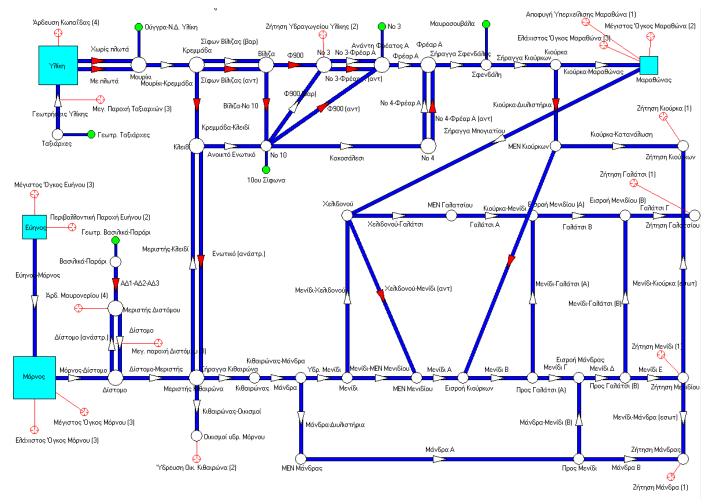
- Find the **maximum possible annual reliable release** from the system:
 - □ for a certain (acceptable) reliability (steady state conditions)
 - for a certain combination of the system components and determine the corresponding:
 - optimal operation policy (storage allocation; conveyance allocation; pumping operation)
 - **cost** (in terms of energy; economy; other impacts)
- Find the minimum total cost
 - for a given water demand (less than the maximum possible annual release)
 - for a certain (acceptable) reliability
 - and determine the corresponding:
 - **combination of the system components** to be enabled
 - optimal operation policy (storage allocation; conveyance allocation; pumping operation)
 - alternative operation policies (that can satisfy the demand but with higher cost)

Categories of problems

- Steady state problems for the current hydrosystem
 - (e.g. previous slide)
- Problems involving time
 - Availability of water resources in the months to come
 - Impact of a management practice to the future availability of water resources
 - Evolution of the operation policy for a temporally varying demand
- Investigation of scenarios
 - Hydrosystem structure: Impacts of new components (aqueducts, pumping stations etc.)
 - Demand: Feasibility of expansion of domain
- Adequacy/safety under exceptional events Required measures
 - Damages
 - Special demand occasions (e.g. 2004 Olympic Games)

Control variables – Parameterization

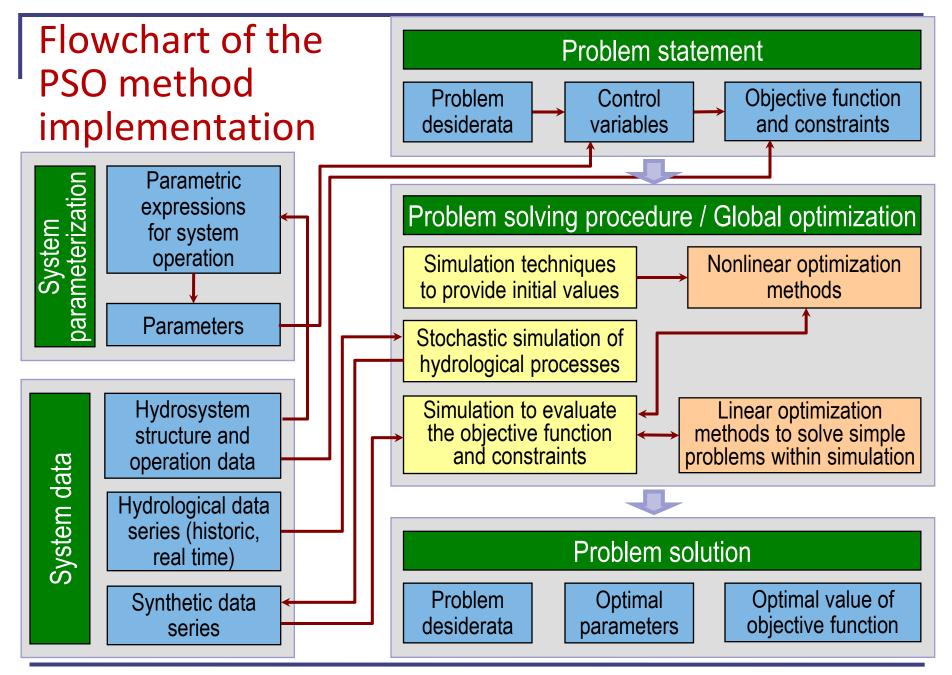
We assume a control horizon of 10 years and monthly scale of simulation; the network includes 60 branches



Number of control variables: According to a conventional approach: 1 variable/ branch/month × 60 branches × 120 months =7200 According to the PSO approach: 4 reservoirs $\times 2$ parameters/ reservoir = 8

Simulation and optimization

- Assuming that parameters a_i and b_i of the operation rule are known, the target releases from each reservoir will be also known at the beginning of each simulation time step
- The actual releases depend on several attributes of the hydrosystem (physical constraints)
- Their estimation is done using simulation
- Within simulation, an internal optimization procedure may be necessary (typically linear, nonparametric)
- Because parameters a_i and b_i are not known, but rather are to be optimized, simulation is driven by an external optimization procedure (nonlinear)



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Milestones in the development of the methodology and the software system

Project initiation: 1999

First master plan of the hydrosystem: Koutsoyiannis et al. (2000)

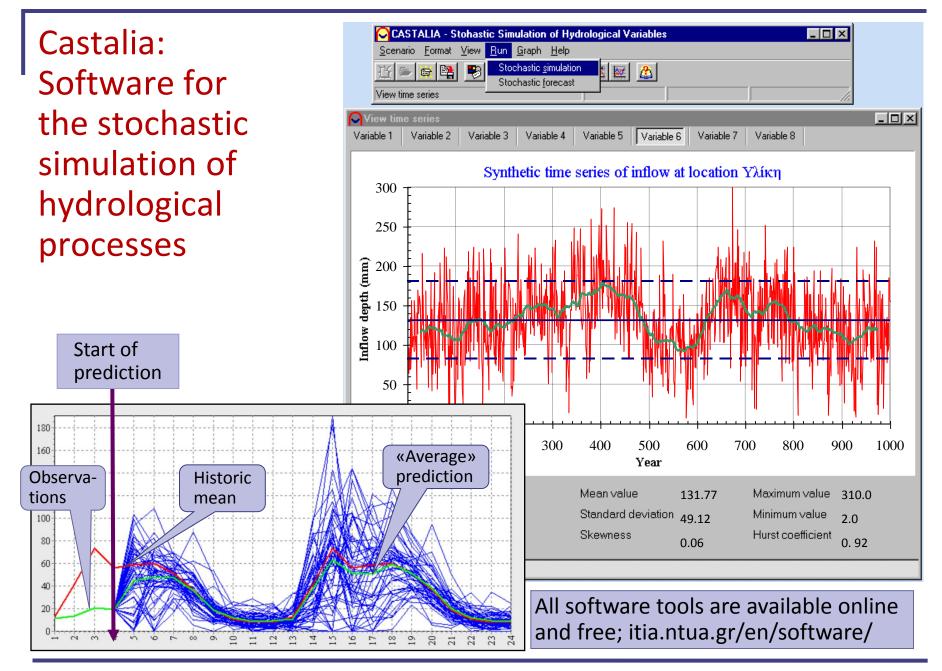
Completion of a decision support tool: Nalbantis et al. (2004)



Hydrognomon: Software for the management and processing of hydrological data

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All software tools are available online and free; itia.ntua.gr/en/software/ See also poster A121 at the Session on *Open Source Computing in Hydrology* (25 Apr 17:30–19:00)



Hydronomeas: Software for hydrosystem optimization

Φόρμα	Κόμβου/Ταμιευτήρα	🛛 Φόρμα Υδραγο	νγείου	×	Φόρμα Γεώτρησης 🛛 🗵
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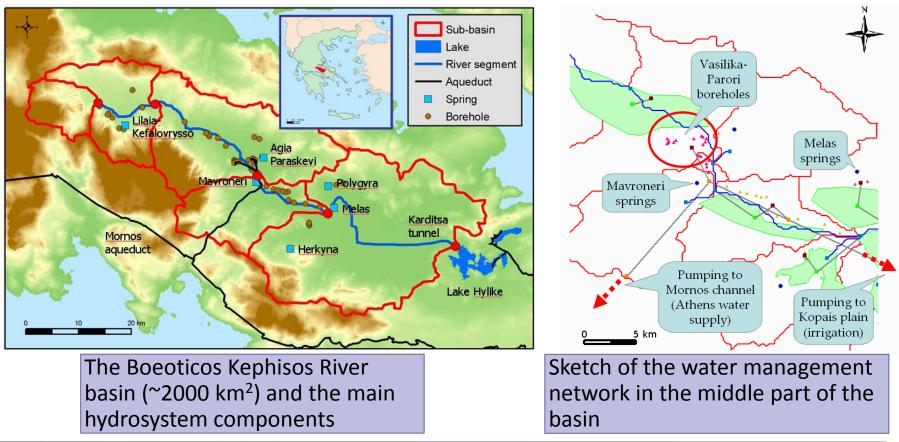
D. Koutsoyiannis, A Monte Carlo approach to water management 39

A human-modified inadequately measured basin: hydrological model calibration and water management

See details in: Efstratiadis et al. (2008); Nalbantis et al. (2011)

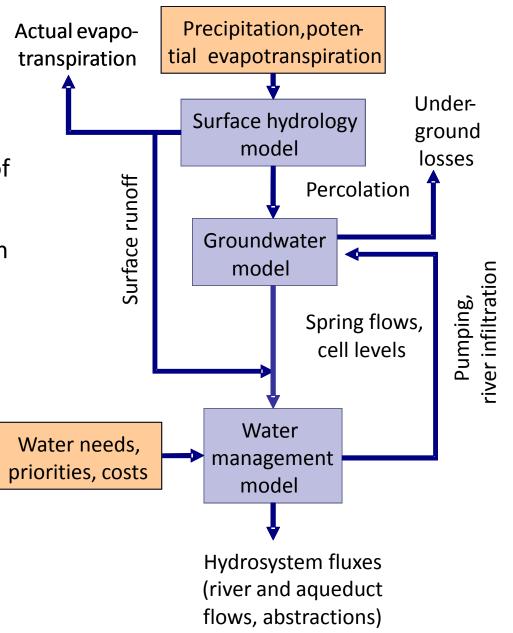
The Boeoticos Kephisos hydrosystem

- Domination of groundwater flow (karst area)
- High withdrawal of groundwater—but not measured
- Modelling of surface water and groundwater flows cannot be separated from each other and from a water management model

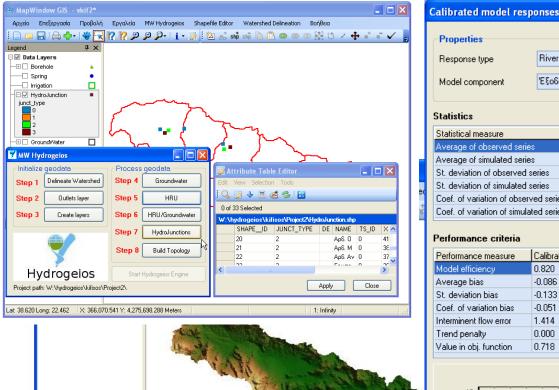


Different problem objectives dealt with using the PSO method

- Parameters of hydrological models along with parameters of the operation rules (concerning the unknown past surface and groundwater withdrawals, which affect measured flows) are determined by the PSO method
 - The objective function is related to the fitting of the model outputs with observations
- Search of optimal designs and future management policies are again determined by the PSO method
 - The objective function is related to the cost and the reliability of the system



Hydrogeios: Software for holistic river basin simulation



Lat: 39.011 Long: 22.474

Preview Map

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X: 367,877.883 Y: 4,319,133.866 Meters

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Value in obj. function 0.718 1.404 Iouii-86 0.000 0.000
Discharge (m3/s)

All software tools are available online and free; itia.ntua.gr/en/software/

Instead of conclusions

Classical approach	Inconsistency	New approach
Input time series are known	Water management is made with reference to the future, which is unknown	The parameters of a stochastic (Monte Carlo) model of inflows are known
Control variables are the controlled water fluxes per time step	This results in inflationary modelling which contravenes the principle of parsimony and is meaningless due to the uncertain future	The parameterization approach, in which the control variables are the parameters of operation rules, radically reduces dimensionality
Simplified system representation	Common simplifications (e.g. discretization, avoidance of probabilistic constraints) annuls the optimality of the solutions determined	Faithful system representation and assessment of performance via stochastic (Monte Carlo) simulation
Use of simplified optimization methods, such as linear or dynamic programming	Water management problems are highly nonlinear (except some simple sub-problems); dynamic programming is inappropriate	Nonlinear stochastic (Monte Carlo) optimization

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