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Is deterministic physically-based hydrological modeling a feasible target? Incorporating physical knowledge in stochastic modeling of uncertain systems

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A premise on terminology

Physically-based, spatially-distributed and deterministic are often used as synonyms. This is not correct.

- **Physically-based model: based on the application of the laws of physics.** In hydrology, the most used physical laws are the Newton's law of the gravitation and the laws of conservation of mass, energy and momentum.
- **Spatially-distributed model: model's equations are applied at local instead of catchment scale.** Spatial discretization is obtained by subdividing the catchment in subunits (subcatchments, regular grids, etc).
- **Deterministic model: model in which outcomes are precisely determined** through known relationships among states and events, without any room for random variation. In such model, a given input will always produce the same output



Sir Isaac Newton
(1689, by Godfrey Kneller)



A premise on terminology

Fluid mechanics obeys the laws of physics. However:

- **Most flows** are turbulent and thus **can be described only probabilistically** (note that the stress tensor in turbulent flows involves covariances of velocities).
- Even viscous flows are au fond described in statistical thermodynamical terms macroscopically lumping interactions at the molecular level.

It follows that:

- **A physically-based model is not necessarily deterministic.**

A hydrological model should, in addition to be physically-based, also consider chemistry, ecology, etc.

In view of the extreme complexity, diversity and heterogeneity of meteorological and hydrological processes (rainfall, soil properties...) physically-based equations are typically applied at local (small spatial) scale. It follows that:

- **A physically-based model often requires a spatially-distributed representation.**

A premise on terminology

In fact, **some uncertainty** is always present in hydrological modeling. **Such uncertainty is** not related to limited knowledge (epistemic uncertainty) but is rather **unavoidable**.

It follows that **a deterministic representation is not possible in catchment hydrology**.

The most comprehensive way of dealing with uncertainty is statistics, through the theory of probability.

Therefore **a stochastic representation is unavoidable in catchment hydrology** (sorry for that... 😊).

The way forward is the **stochastic physically-based model**, a classical concept that needs to be brought in new light.

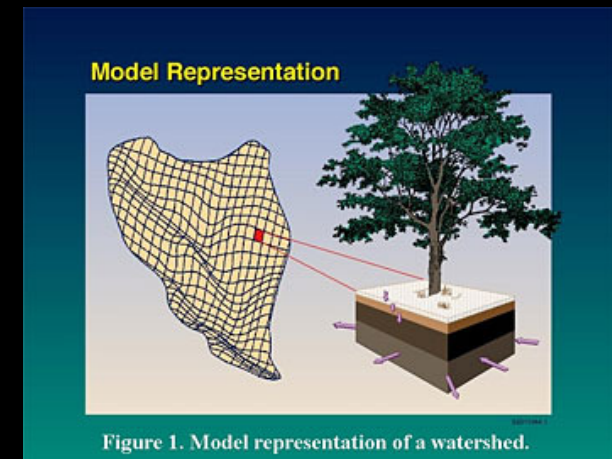


Figure taken from <http://hydrology.pnl.gov/>

Formulating a physically-based model within a stochastic framework

Hydrological model:

in a **deterministic framework**, the hydrological model is usually defined as a **single-valued** transformation expressed by the general relationship:

$$Q_p = S(\boldsymbol{\varepsilon}, \mathbf{I})$$

where Q_p is the model prediction, S expresses the model structure, \mathbf{I} is the input data vector and $\boldsymbol{\varepsilon}$ the parameter vector.

In the **stochastic framework**, the **hydrological** model is expressed in stochastic terms, namely (Koutsoyiannis, 2010):

$$f_{Q_p}(Q_p) = K f_{\boldsymbol{\varepsilon}, \mathbf{I}}(\boldsymbol{\varepsilon}, \mathbf{I})$$

where f indicates the probability density function, and K is a **transfer operator that depends on model S** .

Formulating a physically-based model within a stochastic framework

Assuming a single-valued (i.e. deterministic) transformation $S(\boldsymbol{\varepsilon}, \mathbf{I})$ as in previous slide, the operator K will be the Frobenius-Perron operator (e.g. Koutsoyiannis, 2010).

However, K can be generalized to represent a so-called stochastic operator, which corresponds to one-to-many transformations S .

A stochastic operator can be defined using a stochastic kernel $k(e, \boldsymbol{\varepsilon}, \mathbf{I})$ (with e intuitively reflecting a deviation from a single-valued transformation; in our case it indicates the model error) having the properties

$$k(e, \boldsymbol{\varepsilon}, \mathbf{I}) \geq 0 \quad \text{and} \quad \int_e k(e, \boldsymbol{\varepsilon}, \mathbf{I}) de = 1$$

Formulating a physically-based model within a stochastic framework

Specifically, **the operator K** applying on $f_{\boldsymbol{\varepsilon}, \mathbf{I}}(\boldsymbol{\varepsilon}, \mathbf{I})$ is then **defined as** (Lasota and Mackey, 1985, p. 101):

$$K f_{\boldsymbol{\varepsilon}, \mathbf{I}}(\boldsymbol{\varepsilon}, \mathbf{I}) = \int_{\boldsymbol{\varepsilon}} \int_{\mathbf{I}} k(e, \boldsymbol{\varepsilon}, \mathbf{I}) f_{\boldsymbol{\varepsilon}, \mathbf{I}}(\boldsymbol{\varepsilon}, \mathbf{I}) d\boldsymbol{\varepsilon} d\mathbf{I}$$

If the random variables **$\boldsymbol{\varepsilon}$** and **\mathbf{I}** are **independent**, the model can be written in the form:

$$f_{Q_p}(Q_p) = K [f_{\boldsymbol{\varepsilon}}(e) f_{\mathbf{I}}(\mathbf{I})]$$

$$f_{Q_p}(Q_p) = \int_{\boldsymbol{\varepsilon}} \int_{\mathbf{I}} k(e, \boldsymbol{\varepsilon}, \mathbf{I}) f_{\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}) f_{\mathbf{I}}(\mathbf{I}) d\boldsymbol{\varepsilon} d\mathbf{I}$$

Formulating a physically-based model within a stochastic framework

Estimation of prediction uncertainty:

Further assumptions:

- 1) model error is assumed to be independent of input data error and model parameters.
- 2) Prediction is decomposed in two additive terms, i.e. :

$$Q_p = S(\boldsymbol{\varepsilon}, \mathbf{I}) + e$$

where S represents the deterministic part and the **structural error** e has density $f_e(e)$.

- 3) Kernel independent of $\boldsymbol{\varepsilon}, \mathbf{I}$ (depending on e only), i.e.:

$$k(e, \boldsymbol{\varepsilon}, \mathbf{I}) = f_e(e)$$

By substituting in the equation derived in the previous slide we obtain:

$$f_{Q_p}(Q_p) = \int_{\boldsymbol{\varepsilon}} \int_{\mathbf{I}} f_e(Q_p - S(\boldsymbol{\varepsilon}, \mathbf{I})) f_{\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}) f_{\mathbf{I}}(\mathbf{I}) d\boldsymbol{\varepsilon} d\mathbf{I}$$

Formulating a physically-based model within a stochastic framework

Symbols:

- Q_p true (unknown) value of the hydrological variable to be predicted
- $S(\boldsymbol{\varepsilon}, \mathbf{I})$ Deterministic hydrological model
- e Model structural error
- $\boldsymbol{\varepsilon}$ Model parameter vector
- \mathbf{I} Input data vector

From the deterministic formulation:

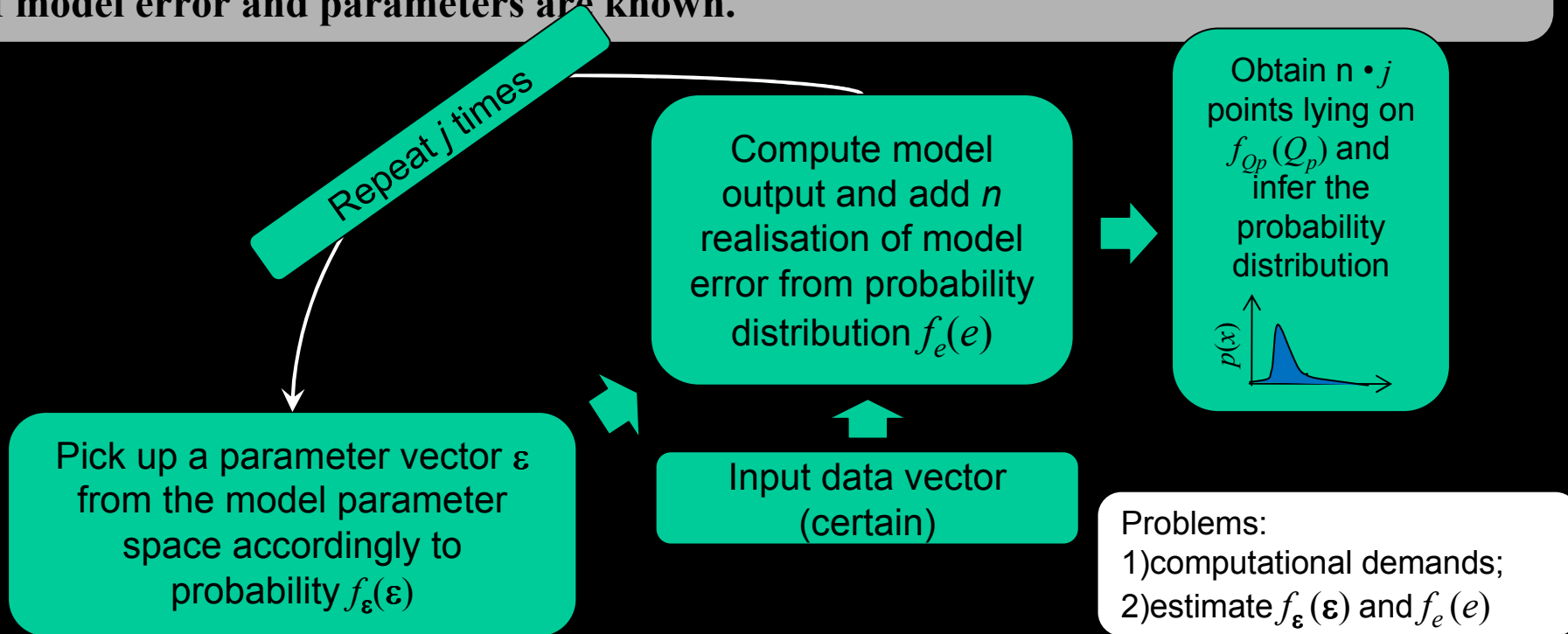
$$Q_p = S(\boldsymbol{\varepsilon}, \mathbf{I})$$

to the stochastic simulation:

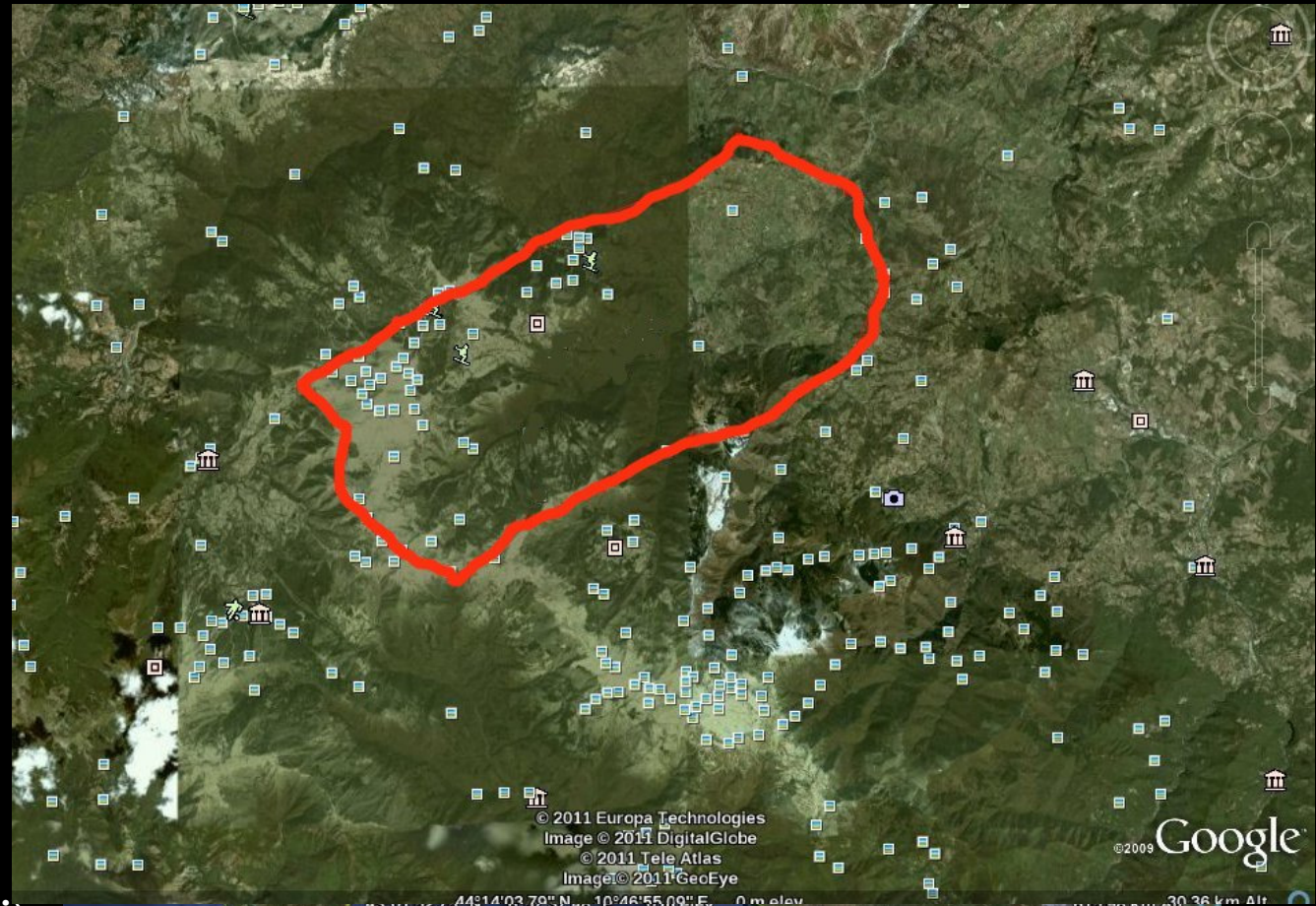
$$f_{Q_p}(Q_p) = \int_{\boldsymbol{\varepsilon}} \int_{\mathbf{I}} f_e(Q_p - S(\boldsymbol{\varepsilon}, \mathbf{I})) f_{\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}) f_{\mathbf{I}}(\mathbf{I}) d\boldsymbol{\varepsilon} d\mathbf{I}$$

Formulating a physically-based model within a stochastic framework

An example of application: model is generic and possibly physically-based. Let us assume that input data uncertainty can be neglected, and that probability distributions of model error and parameters are known.



Example: Leo Creek at Fanano (Italy)



(Courtesy by: Elena Montosi)

This presentation is available for download at the website: <http://www.albertomontanari.it>

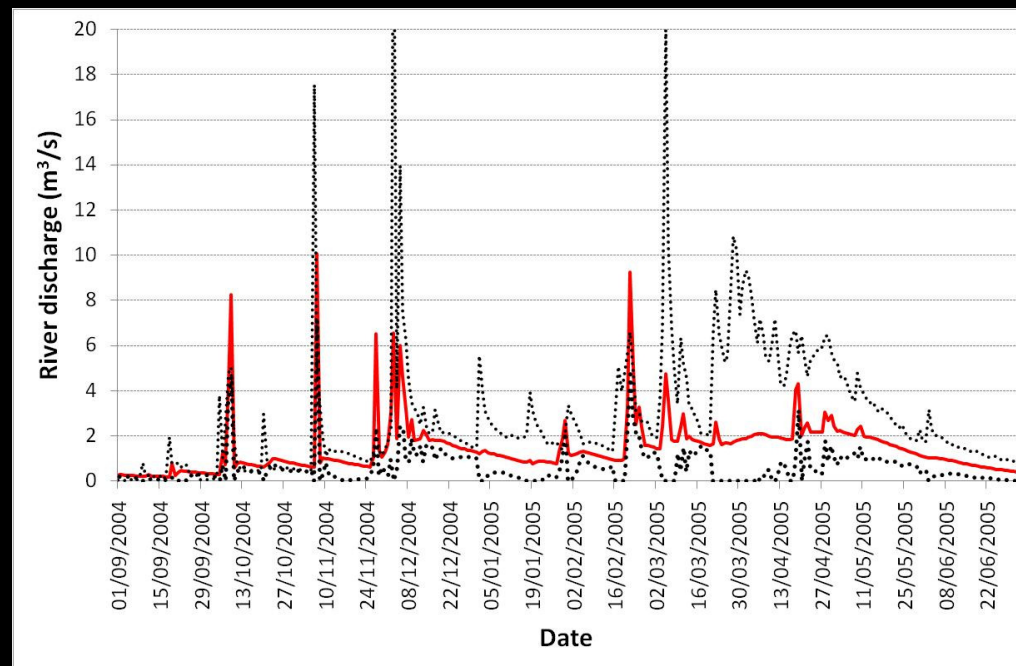
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Estimation of the predictive distribution

Rainfall runoff model: AFFDEF – Daily time scale – Conceptual , 7 parameters

Parameter distribution: estimated by using DREAM (Vrugt and Robinson, 2007)

Generation of random samples of model error: by using the meta – Gaussian approach (Montanari and Brath, 2004; Montanari and Grossi, 2008).





Research challenges

To include a **physically-based model** within a **stochastic framework** is in principle easy. Nevertheless, relevant research challenges need to be addressed:

- **numerical integration** (e.g. by Monte Carlo method) is **computationally intensive** and may result **prohibitive** for **spatially-distributed models**. There is the need to develop efficient simulation schemes;
- a relevant issue is the estimation of **model structural uncertainty**, namely, the estimation of the probability distribution $f(e)$ of the model error. The literature has proposed a variety of different approaches, like the **GLUE method** (Beven and Binley, 1992), the **meta-Gaussian model** (Montanari and Brath, 2004; Montanari and Grossi, 2008), **Bayesian Model Averaging**. For forecasting, Krzysztofowicz (2002) proposed the **BFS method**;
- estimation of **parameter uncertainty** is a relevant challenge as well. A possibility is the **DREAM** algorithm (Vrugt and Robinson, 2007).



Concluding remarks

- A **deterministic representation is not possible in hydrological modeling**, because uncertainty will never be eliminated. Therefore, **physically-based models need to be included within a stochastic framework**.
- The complexity of the modeling scheme increases, but **multiple integration** can be easily approximated with **numerical integration**.
- The **computational requirements** may become **very intensive** for spatially-distributed models.
- How to efficiently assess **model structural uncertainty** is still a relevant research challenge, especially for ungauged basins.
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