



Universiteit Utrecht  Stochastic Hydrology

# Forward stochastic modelling

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## The problem of stochastic forward modelling

- Discharge calculated from water height over a weir subject to error
- Groundwater head from (partly) unknown conductivity
- Concentration of a lake using a decay rate that is not exactly known

Input or parameters  $Z$ , model output  $Y$ , function or model  $g()$ :

$$Y = g(Z)$$

Given the pdf  $f_Z(z)$  of  $Z$  or its moments (mean, variance),  
 What is the pdf  $f_Y(y)$  of  $Y$  or its moments?



## The problem of stochastic forward modelling

Which method to use depends on:

- the form of  $g()$ ;
- what is known about  $Z$ , the complete pdf or its moments.



## Classification of methods

Classification of problems:

- explicit functions of one random variable ←
- explicit functions of multiple random variables ←
- explicit vector functions
- explicit functions of random functions of time, space or space-time
- differential equations with a random parameter ←
- stochastic differential equations ←



## Explicit functions of one random variable

Explicit function:  $Y = g(Z)$

Implicit function:  $Y = g(Z, Y)$  Includes differential equations



## Explicit functions of one random variable

Method 1: Derived distribution

Goal:

- the probability density function  $f_Y(y)$ .

Requirements:

- the probability density  $f_Z(z)$  of  $Z$  is known;
- the function  $g(Z)$  is monotonous (only increasing or only decreasing), differentiable and can be inverted.

Cumulative distribution function:  $F_Y(y) = F_Z(g^{-1}(y))$

Probability density function:  $f_Y(y) = \left| \frac{d[g^{-1}(y)]}{dy} \right| f_Z(g^{-1}(y))$



## Explicit functions of one random variable

Method 1: Derived distribution: example

Discharge formula of a weir:  $Q = aH^b$

$$\text{Inverse: } g^{-1}(q) = \left(\frac{q}{a}\right)^{\frac{1}{b}} \longrightarrow F_Q(q) = F_H\left(\left(\frac{q}{a}\right)^{\frac{1}{b}}\right)$$

$$\text{Derivative of inverse: } \frac{dg^{-1}(y)}{dy} = \frac{1}{b} \left(\frac{q}{a}\right)^{\frac{1-b}{b}}$$

$$\longrightarrow f_Q(q) = \frac{1}{b} \left(\frac{q}{a}\right)^{\frac{1-b}{b}} f_H\left(\left(\frac{q}{a}\right)^{\frac{1}{b}}\right)$$



## Explicit functions of one random variable

Method 2: Taylor approximation

Goal:

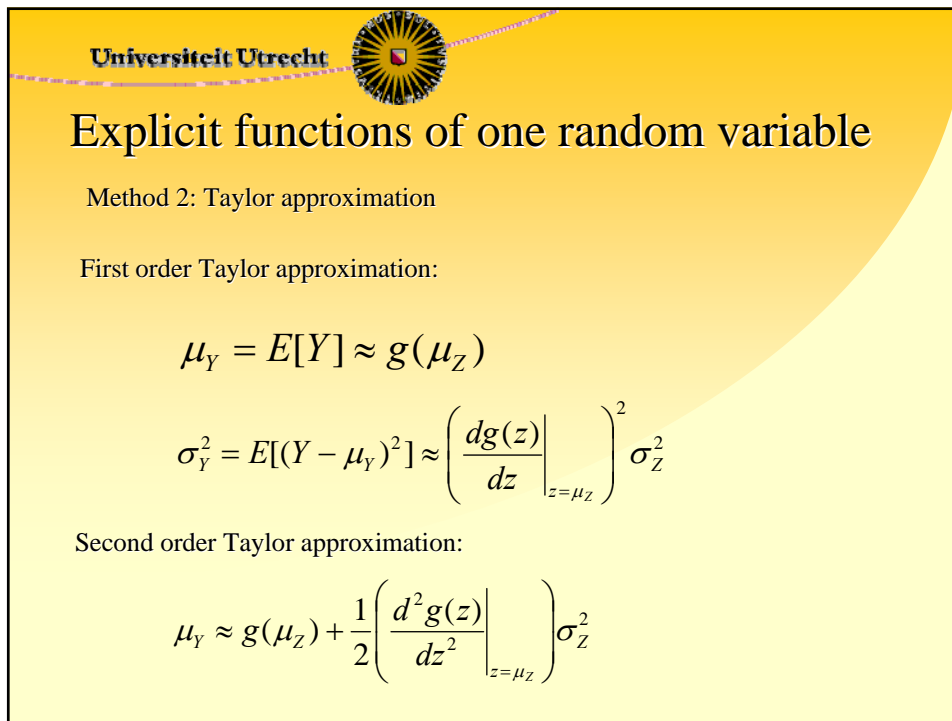
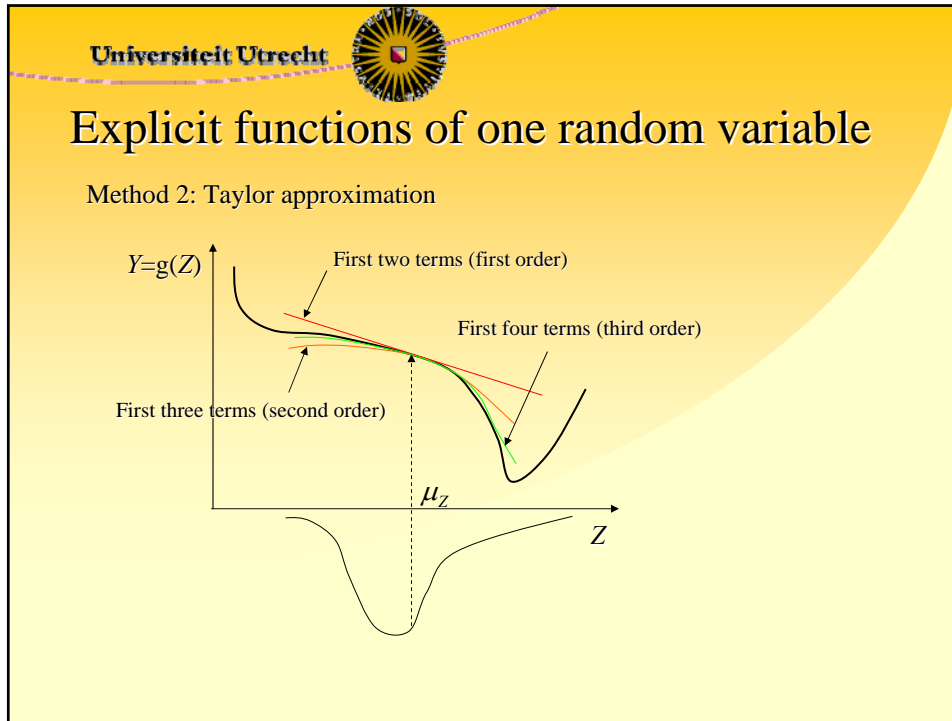
- the moments of  $Y$ , e.g.  $\mu_Y$  and  $\sigma_Y^2$ .

Requirements:

- the moments of  $Z$ , e.g.  $\mu_Z$  and  $\sigma_Z^2$ , are known;
- the variance  $\sigma_Z^2$  should not be too large.
- the function  $g()$  is differentiable

$$Y = g(Z) = g(\mu_Z) + \left(\frac{dg(z)}{dz}\bigg|_{z=\mu_Z}\right)(Z - \mu_Z) +$$

$$\frac{1}{2} \left(\frac{d^2g(z)}{dz^2}\bigg|_{z=\mu_Z}\right)(Z - \mu_Z)^2 + \frac{1}{6} \left(\frac{d^3g(z)}{dz^3}\bigg|_{z=\mu_Z}\right)(Z - \mu_Z)^3 + \dots$$





## Explicit functions of one random variable

Method 2: Taylor approximation: example

Discharge formula of a weir:  $Q = aH^b$

$$\left( \frac{dg(z)}{dz} \Big|_{z=\mu_z} \right) = abh^{b-1} \Big|_{h=\mu_H} = ab\mu_H^{b-1}$$

$$\left( \frac{d^2g(z)}{dz^2} \Big|_{z=\mu_z} \right) = ab(b-1)h^{b-2} \Big|_{h=\mu_H} = ab(b-1)\mu_H^{b-2}$$



## Explicit functions of one random variable

Method 2: Taylor approximation: example


First order Taylor approximation:

$$\mu_Q \approx a\mu_H^b$$

$$\sigma_Q^2 \approx a^2 b^2 \mu_H^{2b-2} \sigma_H^2$$

Second order Taylor approximation:

$$\mu_Q \approx a\mu_H^b + \frac{1}{2} ab(b-1)\mu_H^{b-2} \sigma_H^2$$

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## Explicit functions of one random variable

Method 3: Monte Carlo Simulation


Goal:

- the probability density function or its moments.

Requirements:

- the probability density of  $Z$  is known

No requirements on pdf or form of  $g(Z)$ !

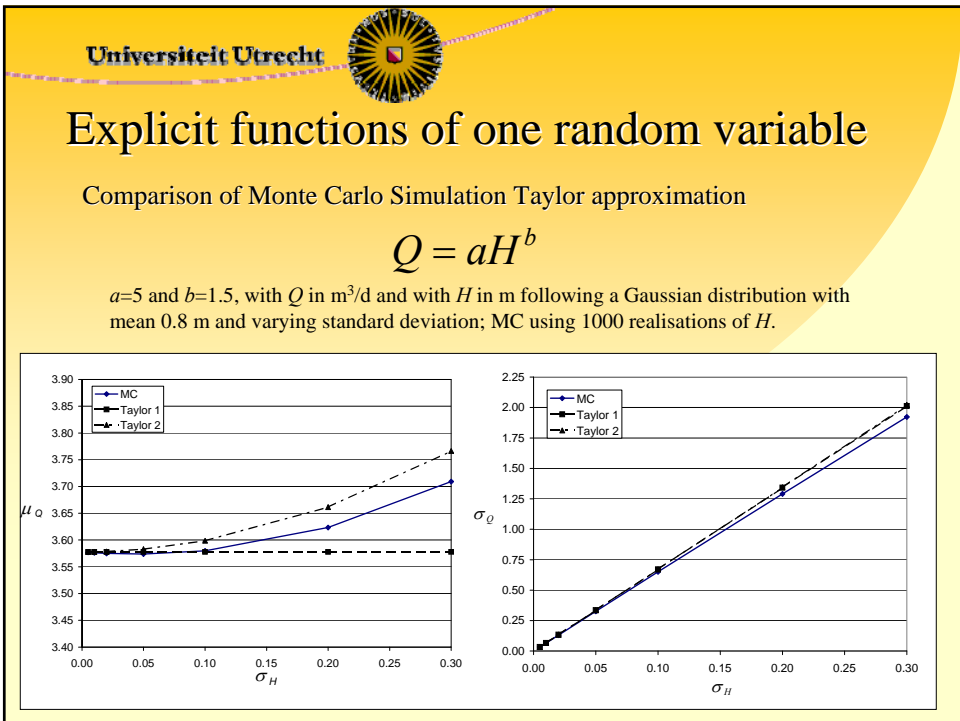
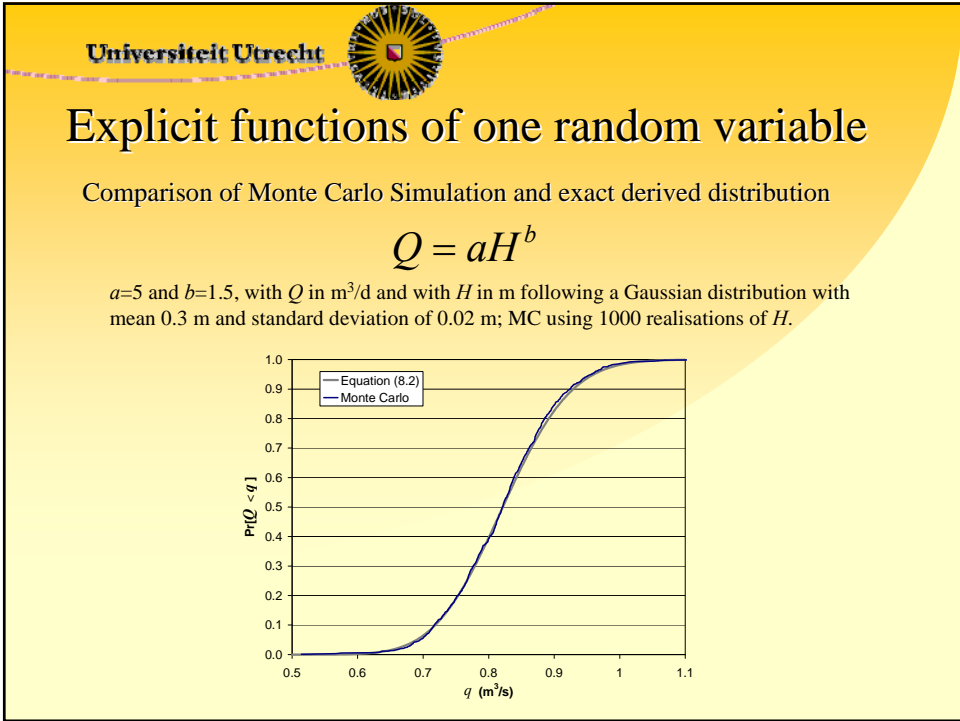
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## Explicit functions of one random variable

Method 3: Monte Carlo Simulation

$u_i$  from uniform[0,1]

The diagram illustrates the transformation of a uniform random variable into a random variable with a specific distribution. On the left, a graph of the cumulative distribution function  $F_Z(z)$  is shown. A horizontal red line at height  $u_i$  intersects the curve, and a vertical red line drops from that point to the  $z$ -axis at  $z_i$ . An arrow labeled  $z_1, \dots, z_M$  points from this graph to a central box labeled  $g(z)$ . Another arrow labeled  $y_1, \dots, y_M$  points from the box to a second graph on the right, which shows the cumulative distribution function  $F_Y(y)$ .







## Explicit functions of multiple random variables

$$Y = g(Z_1, \dots, Z_m)$$

Method 1: linear modelling

Goal:

- the first two moments of  $Y$  .

Requirements:

- the function  $g()$  is linear:  $Y = a + \sum_{i=1}^m b_i Z_i$

Mean: 
$$\mu_Y = a + \sum_{i=1}^m b_i \mu_i$$

Variance: 
$$\sigma_Y^2 = \sum_{i=1}^m \sum_{j=1}^m b_i b_j \rho_{ij} \sigma_i \sigma_j$$

Note: if the  $Z_i$  are multiGaussian then so is  $Y$  and we have the pdf!



## Explicit functions of multiple random variables

Method 2: Taylor approximation

Goal:

- the first two moments of  $Y$  .

Requirements:

- the function  $g()$  is differentiable
- the moments of the  $Z_i$  are known:  $\mu_i, \sigma_i^2, \rho_{ij}$
- the variances  $\sigma_i^2$  are not too large



## Explicit functions of multiple random variables

Method 2: Taylor approximation:

First order mean:

$$\mu_Y = g(\mu_1, \mu_2)$$

Second order mean:

$$\mu_Y = g(\mu_1, \mu_2) + \frac{1}{2} \frac{d^2 g}{dz_1^2}(\mu_1, \mu_2) \sigma_1^2 + \frac{d^2 g}{dz_1 dz_2}(\mu_1, \mu_2) \rho_{12} \sigma_1 \sigma_2 + \frac{1}{2} \frac{d^2 g}{dz_2^2}(\mu_1, \mu_2) \sigma_2^2$$

First order variance:

$$\begin{aligned} \sigma_Y^2 = & g(\mu_1, \mu_2) + \left( \frac{dg}{dz_1}(\mu_1, \mu_2) \right)^2 \sigma_1^2 + \\ & 2 \left( \frac{dg}{dz_1}(\mu_1, \mu_2) \right) \left( \frac{dg}{dz_2}(\mu_1, \mu_2) \right) \rho_{12} \sigma_1 \sigma_2 + \left( \frac{dg}{dz_2}(\mu_1, \mu_2) \right)^2 \sigma_2^2 \end{aligned}$$



## Explicit functions of multiple random variables

Method 2: Taylor approximation:

Example Consider the weir equation or rating curve  $Q = Ah^B$ , where  $A$  and  $B$  are stochastic variables with statistics  $\mu_A, \sigma_A^2, \mu_B, \sigma_B^2$  and  $\rho_{AB}$ . The first order Taylor approximation of the mean becomes:


$$E[Q] \approx \mu_A h^{\mu_B} \quad (8.42)$$

and the second order approximation:

$$E[Q] \approx \mu_A h^{\mu_B} + \frac{1}{2} (\mu_A h^{\mu_B} (\ln h)^2) \sigma_B^2 + (h^{\mu_B} \ln h) \rho_{AB} \sigma_A \sigma_B \quad (8.43)$$

The variance from the first order Taylor analysis is given by:

$$\sigma_Q^2 \approx (h^{2\mu_B}) \sigma_A^2 + (4\mu_A h^{2\mu_B} \ln h) \rho_{AB} \sigma_A \sigma_B + (2\mu_A^2 h^{2\mu_B} (\ln h)^2) \sigma_B^2 \quad (8.44)$$

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## Explicit functions of multiple random variables


Method 3: Monte Carlo simulation

Goal:

- the probability density function or its moments.

Requirements:

- the multivariate probability density of the  $Z_i$  is known

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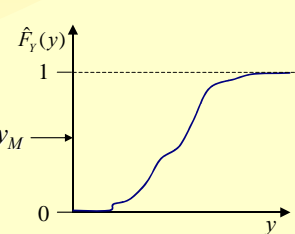
## Explicit functions of multiple random variables

Method 3: Monte Carlo simulation

In practice: the multivariate probability density of the  $Z_i$  is assumed Gaussian  
otherwise: transformation to Gaussians

Generation of  $M$  sets of dependent random variables from multivariate pdf (LU-decomposition)

$\left. \begin{array}{l} \{z_1^{(1)}, z_2^{(1)}, \dots, z_n^{(1)}\} \\ \{z_1^{(2)}, z_2^{(2)}, \dots, z_n^{(2)}\} \\ \vdots \\ \{z_1^{(M)}, z_2^{(M)}, \dots, z_n^{(M)}\} \end{array} \right\} \rightarrow g(z_1, \dots, z_n) \rightarrow y_1, \dots, y_M$





## Differential equation with random coefficients

Example: concentration from a lake  $C$  with time:

$$v \frac{dC}{dt} = -vKC + q_{in}$$

where  $v$  is the volume of the lake (assumed constant and known)  $q_{in}$  is the constant an known input load and  $K$  is a random decay coefficient.

Required: pdf of  $C$  or its moments

Method:

- 1) solve the differential equation (either analytically or numerically) assuming  $K$  deterministic.
- 2) analyse the solution, for the case that  $C$  is random.



## Differential equation with random coefficients

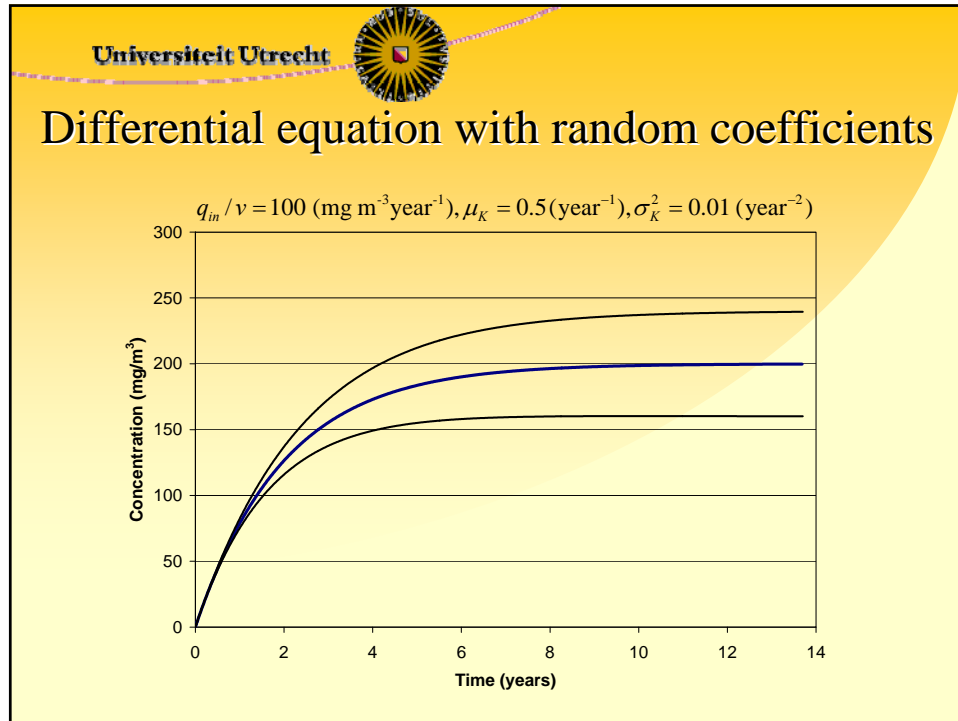
Solution  $C(t=0) = 0$ : 
$$C(t) = \frac{q_{in}}{vK} (1 - e^{-Kt})$$

If moments of  $K$  are known:  $\mu_K, \sigma_K^2$


Perform Taylor approximation or Monte Carlo simulation

First order Taylor approximation of the variance:

$$\sigma_C^2(t) = \frac{q_{in}^2}{v^2} \frac{(e^{-\mu_K t} (1 + \mu_K t) - 1)^2}{\mu_K^4} \sigma_K^2(t)$$



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## Stochastic differential equations

Examples:

1. Evolution of lake concentration with decay rate as a random function of time:
 
$$v \frac{dC}{dt} = -vK(t)C + q_{in}$$
2. Transient groundwater equation for two-dimensional flow with heterogeneous storage coefficient and transmissivity, described as random space functions:
 
$$S(x, y) \frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left( T(x, y) \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y} \left( T(x, y) \frac{\partial H}{\partial y} \right)$$



## Stochastic differential equations

$$v \frac{dC}{dt} = -vK(t)C + q_{in}$$

$$S(x, y) \frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left( T(x, y) \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y} \left( T(x, y) \frac{\partial H}{\partial y} \right)$$

Required, multivariate pdf of  $C$  or  $H$  or its moments:

$$\mu_C(t), \sigma_C^2(t), C_C(t_1, t_2)$$

$$\mu_H(x, y), \sigma_H^2(x, y), C_H(x_1, y_1, x_2, y_2)$$

We cannot solve for deterministic  $S(x, y), T(x, y)$  and  $K(t)$ ,  
and then analyse the solution for randomness!



## Stochastic differential equations

Consider example 2: Concentration pollutant in a lake:

$$\frac{dC}{dt} = -K(t)C + q_{in}c_{in}$$

General solution:

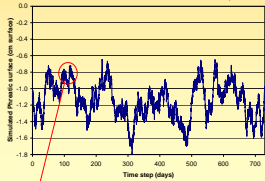
$$C(t) = C(t_0) + q_{in}c_{in}(t - t_0) - \int_0^t CK(t)dt$$

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## Stochastic differential equations

How to solve the stochastic integral:  $\int_0^t CK(t)dt$

Coloured noise



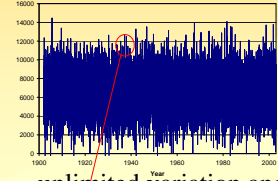
limited variation

$$\text{VAR}[z(t) - z(t + \tau)] \rightarrow 0$$

Smooth at very small scales

Normal calculus

White noise



unlimited variation and infinite variance

$$\text{VAR}[z(t) - z(t + \tau)] \rightarrow \infty$$

Itô calculus

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## Stochastic differential equations

We consider only coloured noise

Solution methods:

a) (Semi-)Analytical derivation of the moments  $\mu_C(t), \sigma_C^2(t), C_C(t_1, t_2)$  as a function of the moments  $\mu_K(t), \sigma_K^2(t), C_K(t_1, t_2)$

- > strict conditions on RF  $K$  (and  $H$  and  $S$ ): stationary and multiGaussian
- > in groundwater flow: uniform flow in infinite domains!
- > small variance  $\sigma_K^2 (\sigma_T^2, \sigma_S^2)$

Examples:

- Small perturbation analysis
- Moment differential equations (usually solved numerically)



## Stochastic differential equations

Solution methods:

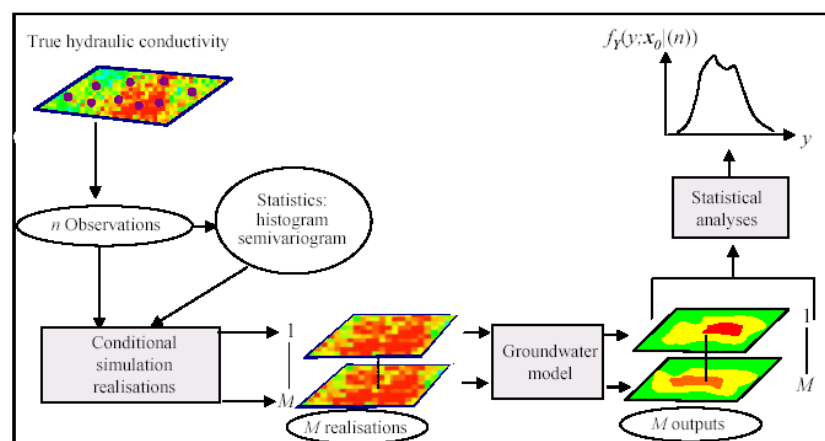
b) Monte Carlo simulation

- required: multivariate pdf of parameters/input
- no additional assumption needed!
- Conditioning on data possible!



## Stochastic differential equations

Monte Carlo simulation: Groundwater example

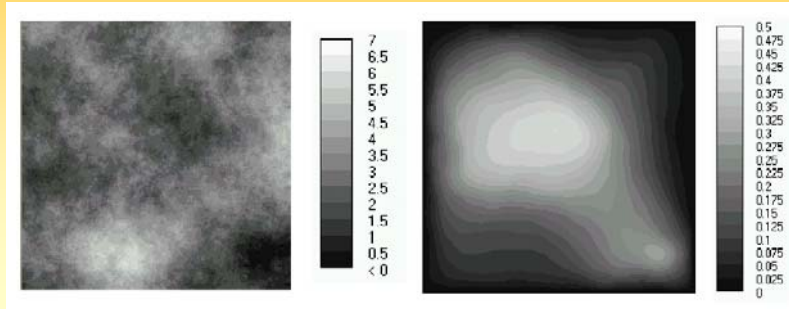






## Stochastic differential equations

Monte Carlo simulation: Groundwater example



Reality. Left: Log-hydraulic conductivity  $Y=\ln K$  ( $K$  in m/d); Right: Hydraulic head (m)

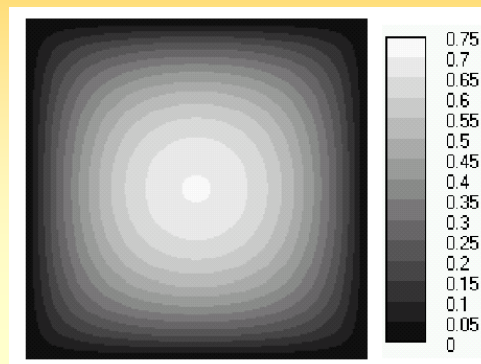
$$K_G = \exp(\mu_Y) = 10 \text{ m/d}; \sigma_Y^2 = 2$$

Hydraulic head at boundaries = 0, precipitation is 1 mm/day.

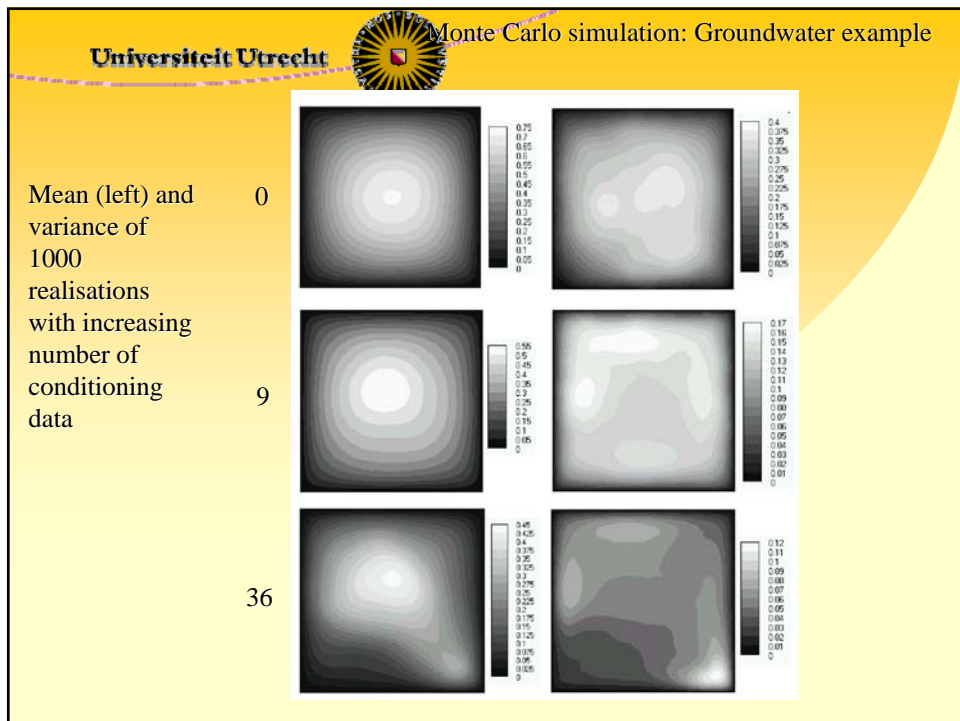
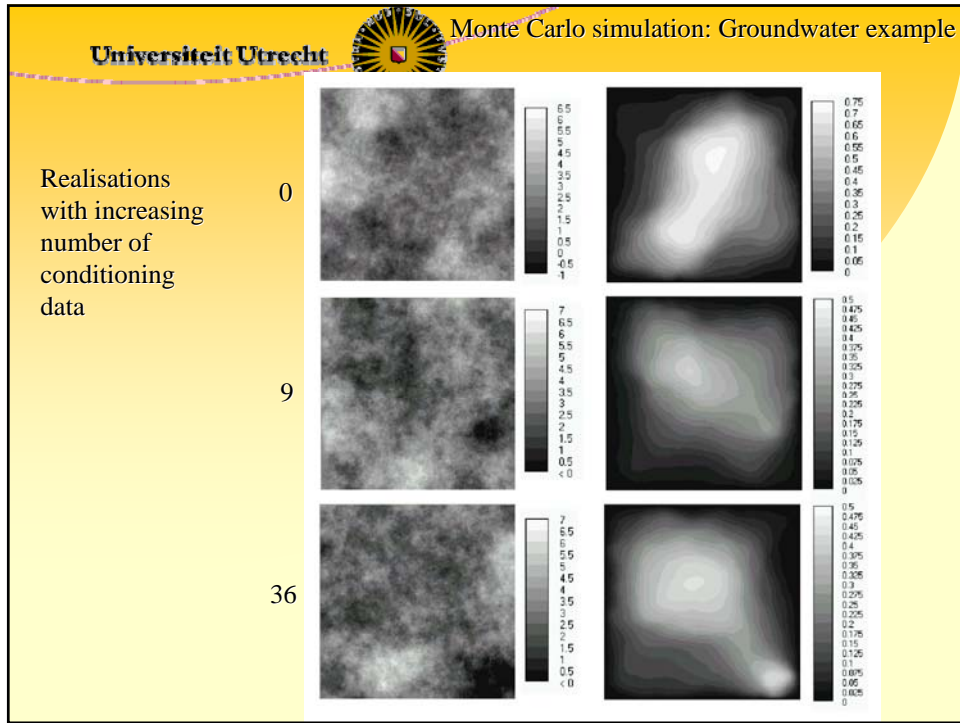


## Stochastic differential equations

Monte Carlo simulation: Groundwater example



Solution assuming homogenous  $K = K_G = 10 \text{ m/d}$ .





### Monte Carlo simulation: Groundwater example

*Relationship between the domain average standard deviation of hydraulic head and the number of observations used for conditioning (zero observations means unconditional simulation)*

