Realistic quantification of input, parameter and structural errors of soil process models

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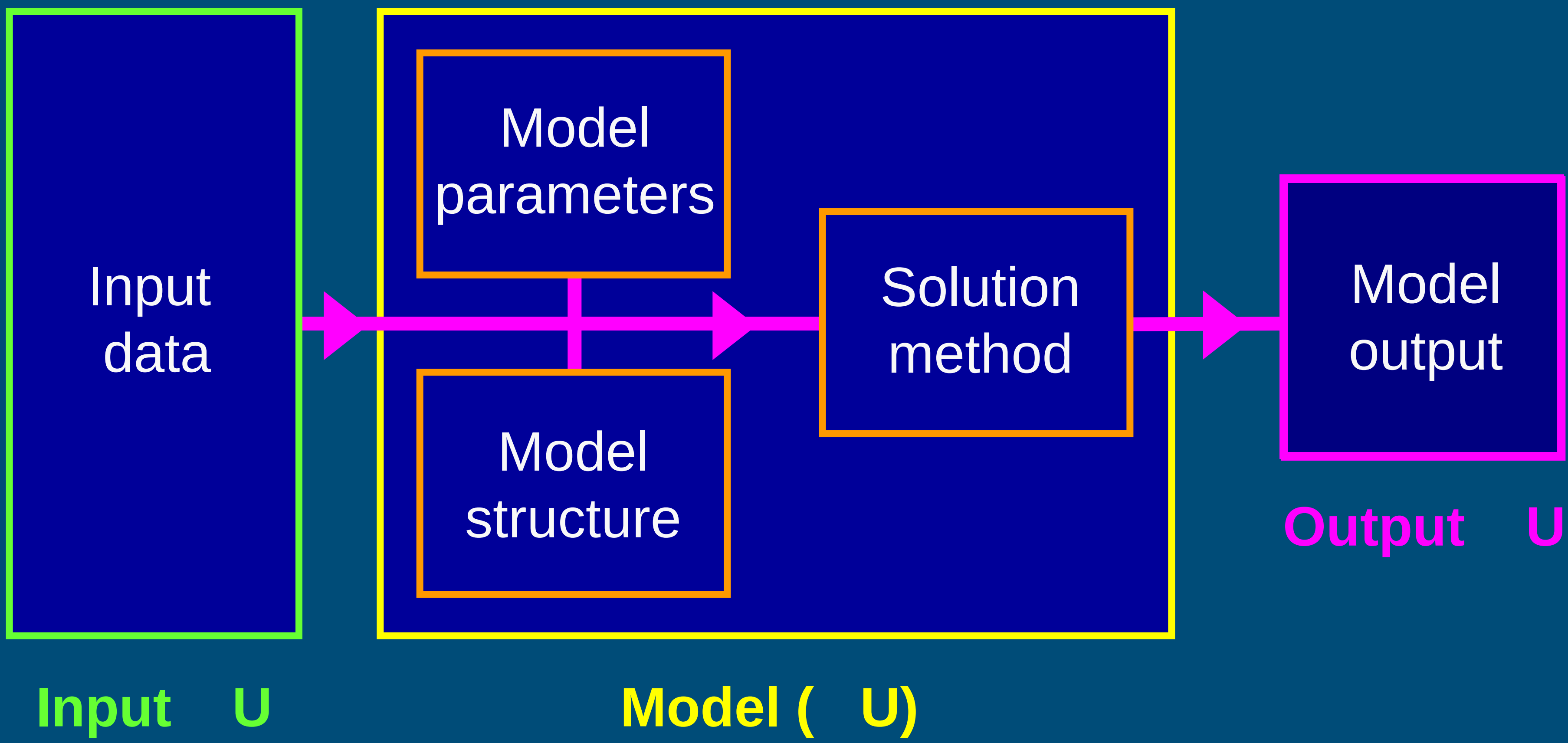
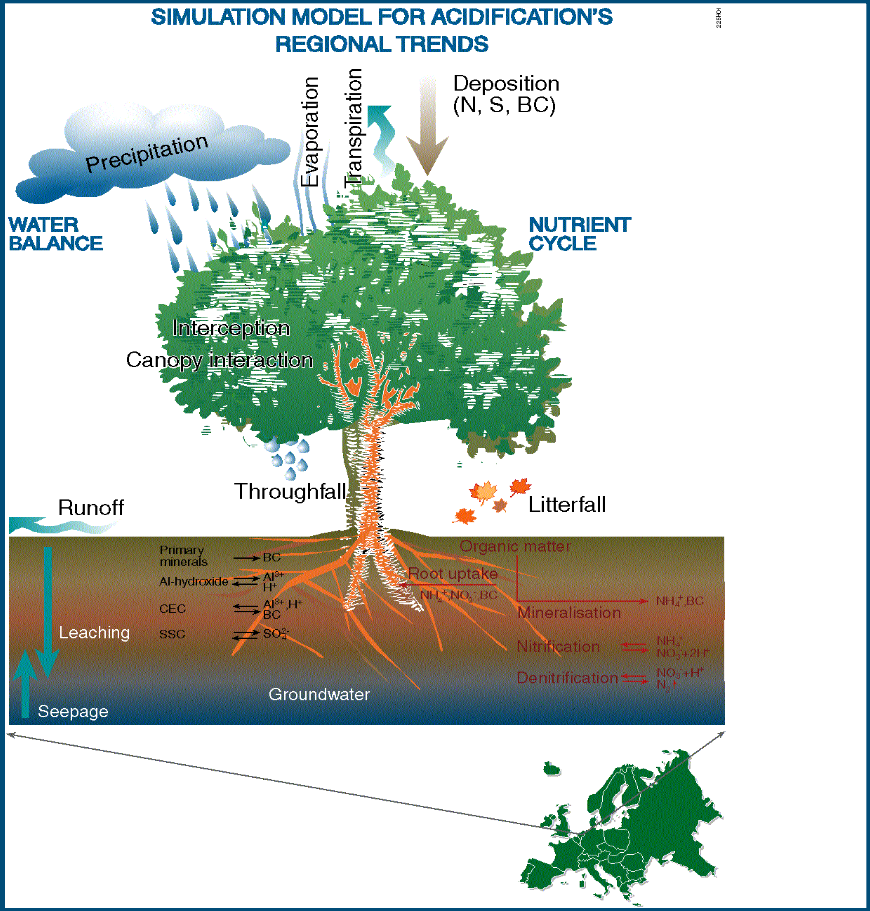
Soil process models are not perfect

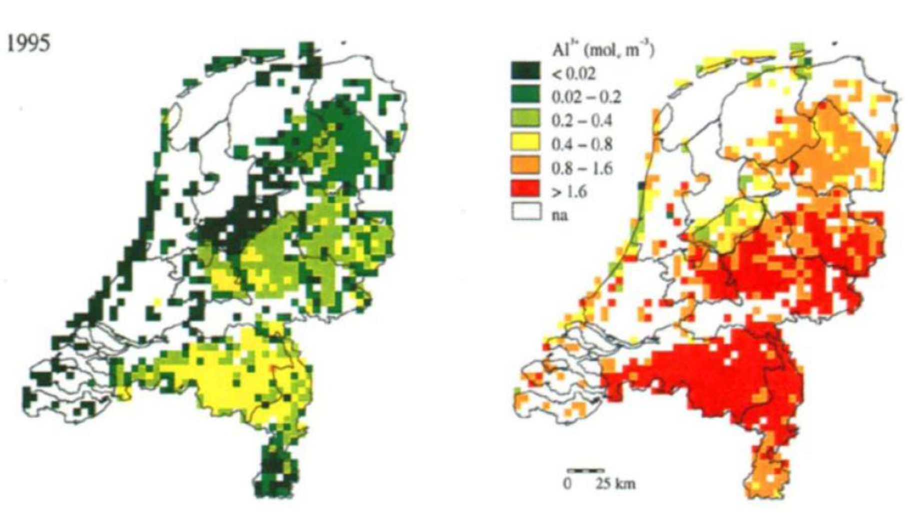


Uncertainty propagation analysis easy once uncertainty sources are quantified by probability distributions

- Monte Carlo method:
  - repeat many times (N>100)
    - generate a realization of the uncertainty sources by sampling from their probability distribution with a random number generator
    - run model and store result for this realization
  - compute and report summary statistics of the N results (e.g. mean, standard deviation, proportion above critical threshold)
- Computationally demanding but flexible, easily implemented and approximation errors can be made arbitrary small

Example: Uncertainty propagation with soil acidification model (Kros et al., JEQ 28, 366-377)





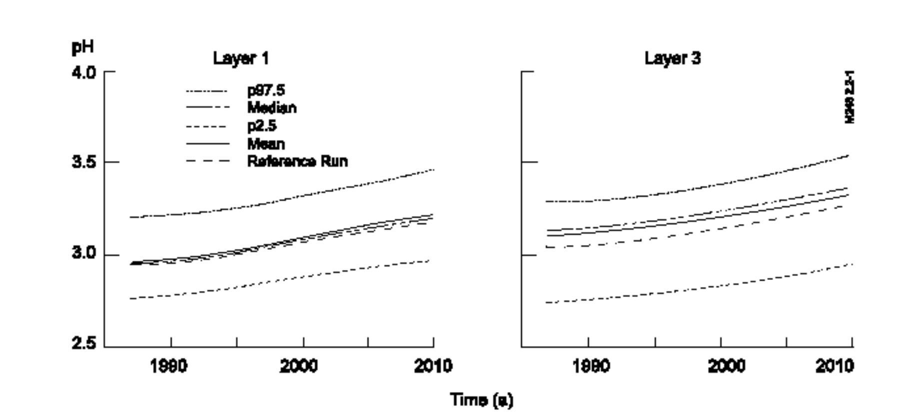


Figure 1 Temporal evolution of the mean, the median, the 97.5 and 2.5 percentiles, and the reference run of the pH in layers 1 and 3.

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Main problem is quantification of uncertainty sources

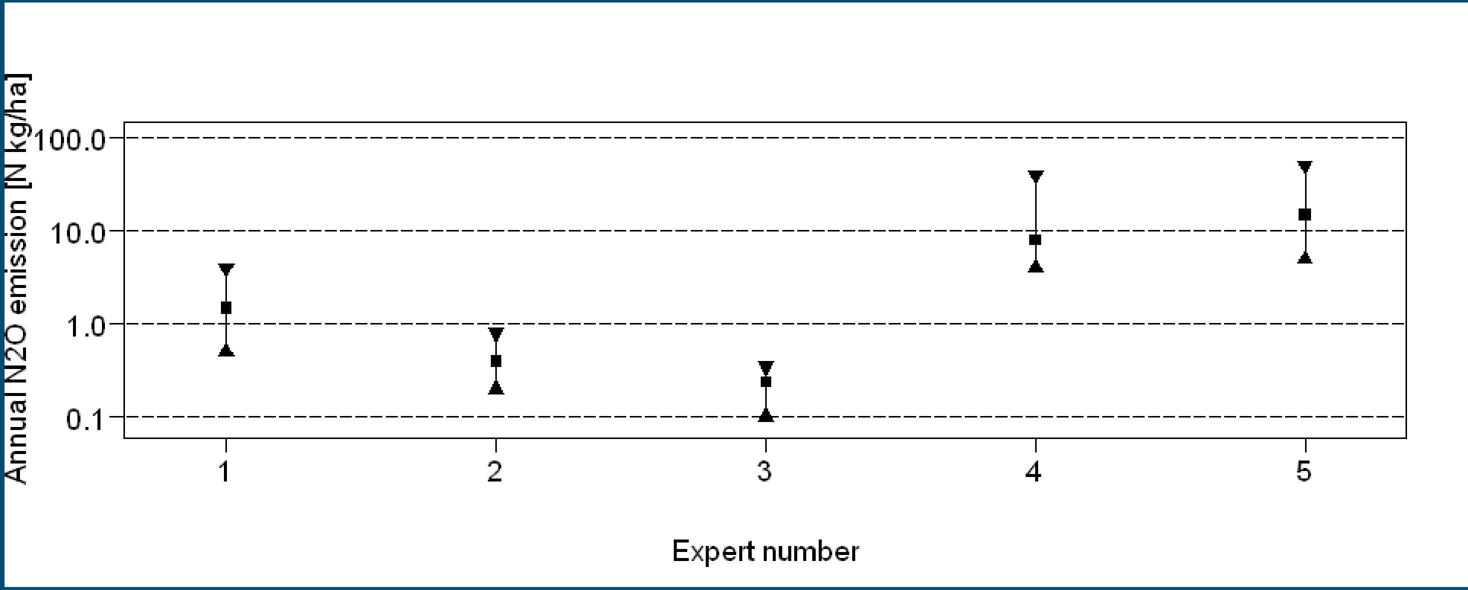
- Single measure of uncertainty (e.g. $X = 10 \pm 2$) is not enough, a full probability distribution function (pdf) is needed:
  - shape of pdf (e.g. normal, lognormal, uniform)
  - parameters of pdf (e.g. mean, standard deviation, skewness)
  - cross-correlations between uncertain inputs or parameters (e.g. uncertainties in clay and sand content are correlated)
  - spatial correlation for uncertain inputs or parameters that vary in space (e.g. by a semivariogram)
  - temporal correlation for variables that vary in time (e.g. correlogram)
- Note that pdf is support-dependent (e.g. uncertainty about OM of 1 cm^3 volume different from that of a 1 dm^3 volume)
- pdf for categorical variables more complex (e.g. soil type)
- pdf required for 1) model inputs; 2) model parameters and 3) model structure

Uncertainty quantification of model inputs

- Many options:
  - measurement error from instrument and lab specifications or by taking replicates
  - sampling error using sampling theory from statistics (e.g. standard error of the mean, confidence intervals)
  - use of ground truth verification data (e.g. soils data base, independent data)
  - interpolation error using geostatistics (kriging variance)
  - errors in transfer functions such as regression: R-square, residual variance, variance of regression coefficients (e.g. pedo-transfer functions)
  - classification error using multivariate statistics (e.g. maximum likelihood classification of remote sensing imagery)
  - input that is output of another model in a model chain: use Monte Carlo sample of output from the other model
  - expert judgement (last resort?)

Uncertainty quantification of model inputs

- In spite of the many options, expert judgement is often used
- Expert judgement of uncertainties often done in an improvised and ad hoc way
- Experts may disagree:



- Let us test how well you can quantify **your uncertainty**

Predicting soil organic matter (mass percentage) of topsoil (0-30 cm) for the Dutch province of Drenthe*

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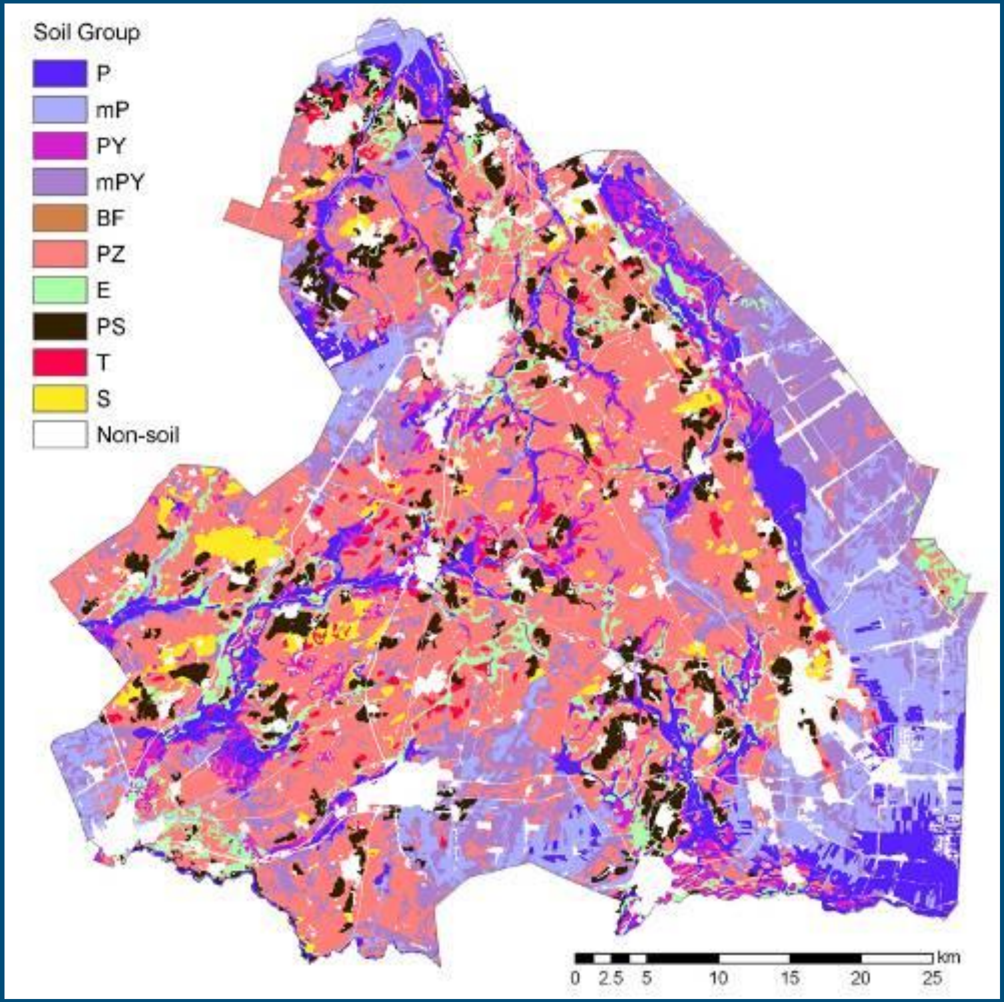
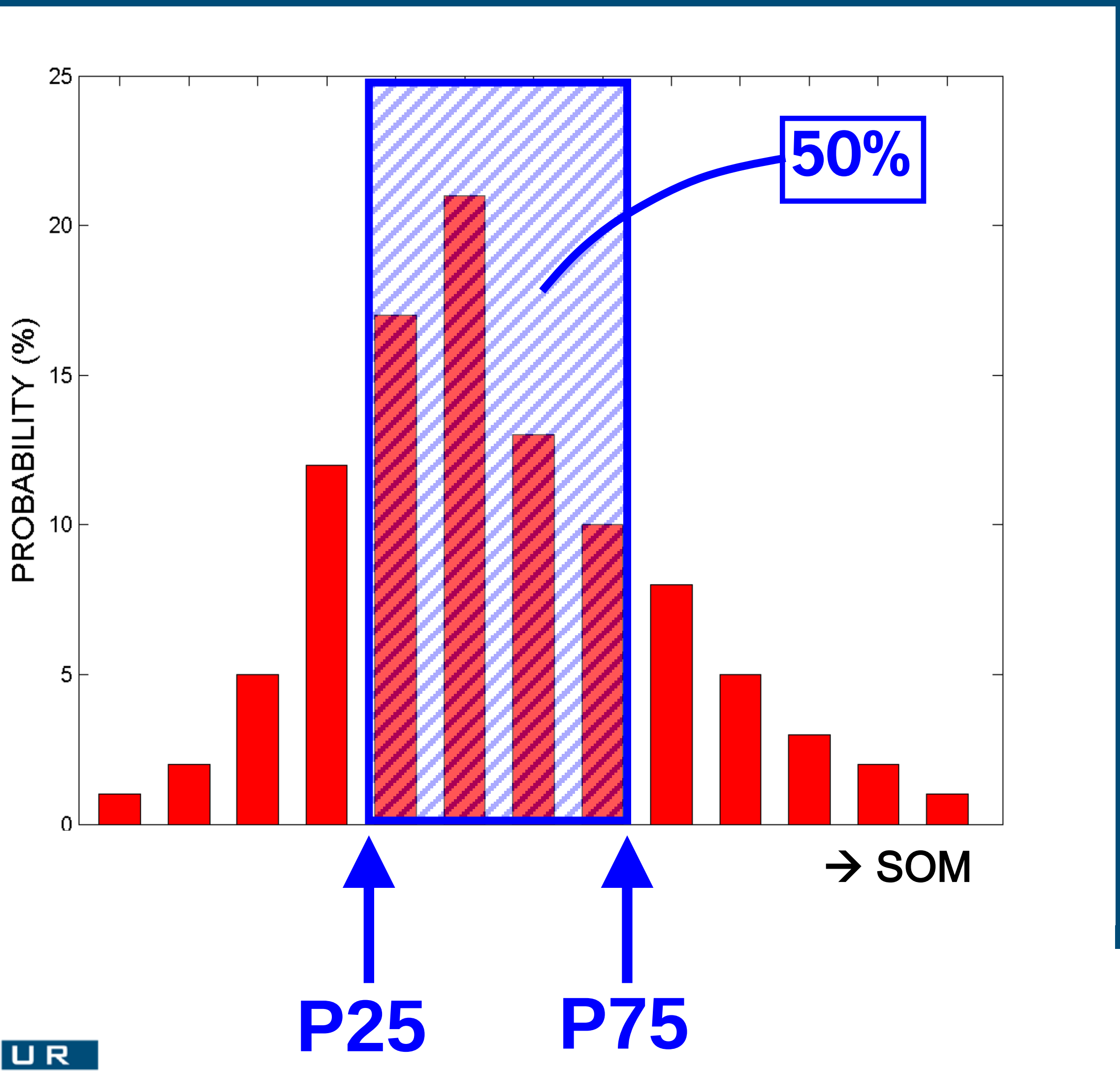
*Data provided by Bas Kempen, thanks!

Soil map of Drenthe shows that the province has peat and mineral (sandy) soils



P = thick peat soils with peaty topsoil; ***mP*** = thick peat soils with mineral topsoil; ***PY*** = thin peat soils with peaty topsoil; ***mPY*** = thin peat soils with mineral topsoil; ***BF*** = brown forest soils; ***PZ*** = podzols; ***E*** = dark hydromorphic earth soils; ***PS*** = plaggen soils; ***T*** = glacial till soils; ***S*** = raw sand soils

Quantify uncertainty with lower and upper limits of the symmetric 50% credibility interval: 50% chance that true value lies in interval



Please stand up

Location 1

0 - 30 cm

Lower limit P25: X %

Upper limit P75: Y %

True value: **21.4** %

Location 2

0 - 30 cm

Lower limit P25: X %

Upper limit P75: Y %

True value: **5.0** %

Location 3

Lower limit P25: X %

Upper limit P75: Y %

True value: **62.6** %

Location 4

0 - 30 cm

Lower limit P25: X %

Upper limit P75: Y %

True value: **8.1** %

Location 5

0 - 30 cm

Lower limit P25: X %

Upper limit P75: Y %

True value: **2.3** %

Location 6

0 - 30 cm

Lower limit P25: X %

Upper limit P75: Y %

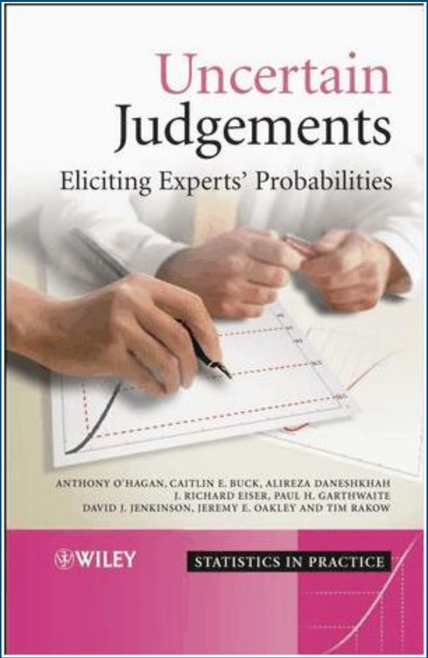
True value: **6.8** %

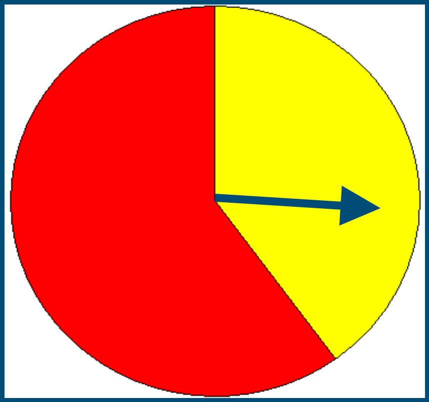
If there had been 64 people in this room....

- Then after location 1 about 32 people still standing
- 2 → 16, 3 → 8, 4→ 4, 5 → 2, 6 → 1
- People that had to sit down immediately tend to be overconfident (type MACHO)
- People that kept standing until the end are too insecure (type SISSY)
- It turns out to be difficult to quantify your own uncertainty
- Need for valid and sound approach: **expert elicitation**

Expert elicitation

- Aims to construct a probability distribution that properly represents the expert's knowledge
- Scientific field in its own right, many text books, conferences and journals
- Involves contributions from statistics and psychology (understanding human judgement)
- Experts must first be calibrated (corrected for over- and underconfidence)
- Elicitation typically proceeds by moving from probabilities to distributions
- If there are multiple experts then distributions must be combined, either by mathematical aggregation or by behavioural aggregation
- Uses formal procedures, also implemented in software tools (e.g. Elicitator from QUT Brisbane!)
- Extension from univariate to multivariate distributions exists, but spatial and temporal extensions are rare





Uncertainty in model parameters

- Parameters different from inputs because parameters are inseparable from the model (e.g. a regression coefficient)
- Implies that model parameters and their uncertainties can only be assessed using calibration procedures (i.e. inverse modelling)
- Common approaches (e.g. PEST as often used in hydrological modelling) recently surpassed by Bayesian calibration:
  - define a prior pdf $p(\theta)$ for parameter (vector) θ
  - compute posterior $p(\theta|\text{data})$ by applying Bayes' rule:

$$p(\theta \mid \text{data}) \propto p(\theta) \cdot p(\text{data} \mid \theta)$$

  - in practice this is done numerically using Markov chain Monte Carlo simulation
- Bayesian calibration – MCMC is computationally demanding but easily implemented, flexible and yields the full joint distribution of all parameters

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Model structural uncertainty

- Arguably the most difficult uncertainty source, because it is difficult to define a pdf for structural errors
- One possible approach is (Bayesian) model averaging: define multiple competing models, each with a certain probability of being correct:
  - requires multiple models: not easy in soil process modelling
  - risk that models have too much overlap and do not cover the full space of possible models because modellers have the same background and copy from each other
- Alternative approach: good-old stochastic models that represent model structural error by additive (or multiplicative) system noise:

$$Z(x,t) = M(x,t) + \varepsilon(x,t)$$

- System noise can be modelled using common (geo)statistical approaches and optimal prediction of Z(x,t) with uncertainty quantification can be achieved with kriging, (space-time) Kalman filtering or stochastic simulation
- Parameters of system noise can also be estimated using Bayesian calibration: take look at integrated approach

Outline of integrated approach to uncertainty propagation analysis that includes all three sources of uncertainty

$O = f(I, \theta, \tau)$

O=output

f=model

θ=model parameters

I=input

τ=model structural error parameters

$p(O|data)$ derived from $p(I,\theta,\tau|data)$ because f known

$$p(I, \theta, \tau \mid data) = p(I) \cdot p(\theta, \tau \mid I, data)$$

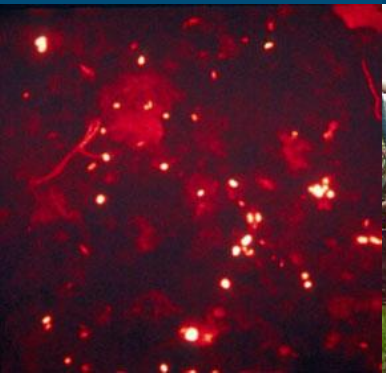
$$p(\theta, \tau \mid I, data) \propto p(\theta, \tau) \cdot p(data \mid I, \theta, \tau)$$

take measurement error into account when specifying $p(data|I,\theta,\tau)$

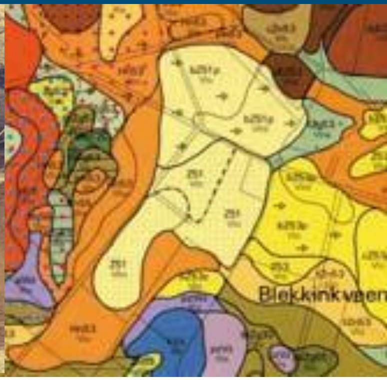
Conclusions

- Uncertainty propagation analysis of soil process models important because:
  - users must know how accurate the results of models are if these results are to be used in decision making
  - information about uncertainty can be used to take better decisions (e.g. risk analysis)
  - it provides insight into how best to improve the accuracy of model output
- Monte Carlo simulation very suitable for uncertainty propagation analysis provided the source uncertainties are quantified with pdfs
- Must use expert elicitation when relying on expert judgement for quantification of input uncertainties
- Bayesian calibration recommended for quantification of uncertainties in model parameters
- Uncertainty about model structure may be described with additive system noise: easy (but perhaps unrealistic and refinement necessary)
- Integrated approach that takes all uncertainty sources into account must be worked out and tested
- Can learn much from related fields such as hydrology and meteorology

Thank you







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