BIOMATH
Department of Applied Mathematics,
Biometrics and Process Control

UNIVERSITEIT
GENT

Integration is a central theme

(Reflections on the SAIA "Specialist" Group)

Peter Vanrolleghem
01-jan-04

Watermatex 2004, Beijing, Nov 3-5 2004

UGent-BIOMATH, Coupure 653, 9000 Gent, Belgium (e-mail Peter.Vanrolleghem@ugent.be)
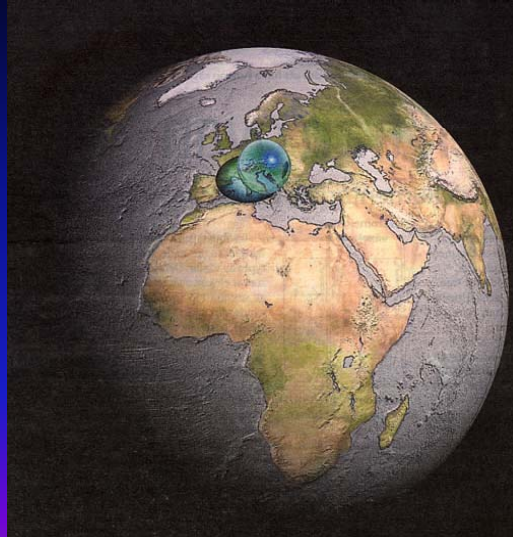

Water…

I begynnelsen skapade Gud himmel och jord. Jorden var öde och tom, och mörker var över djupet. Och Guds Ande svävade över vattnet. *(Genesis 1:1-2)*

In the beginning God created the heaven and the earth. And the earth was without form, and void; and darkness was upon the face of the deep. And the Spirit of God moved upon the face of the waters. *(Genesis 1:1-2)*

Docentföreläsning Ulf Jeppsson, 15 Dec 2003

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Noah's ark flood (5500 B.C.)

Global "Bluewater" Resources
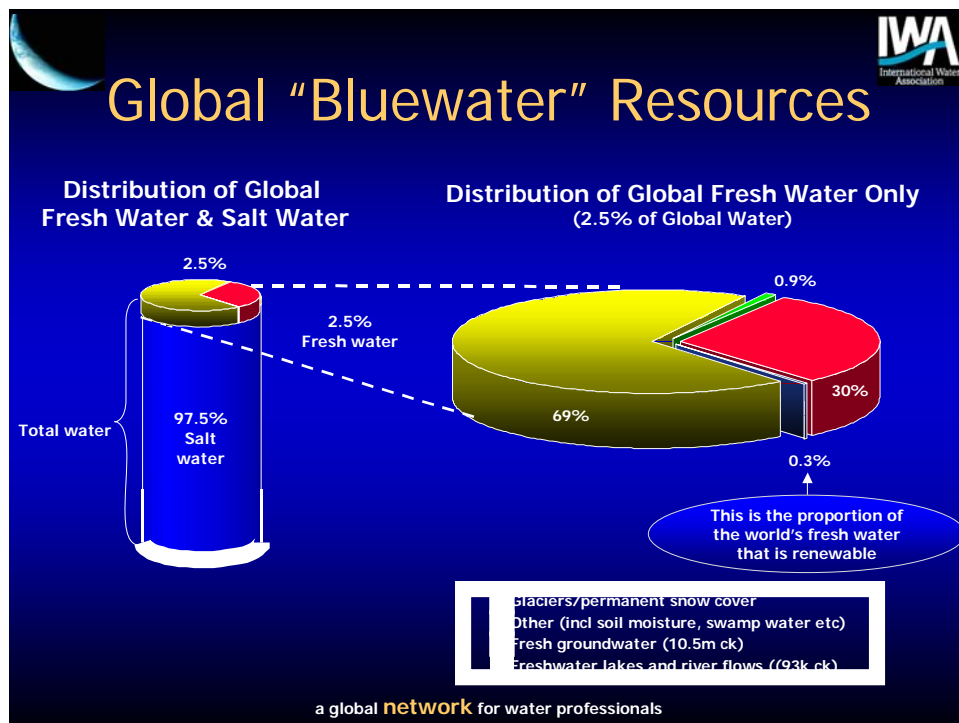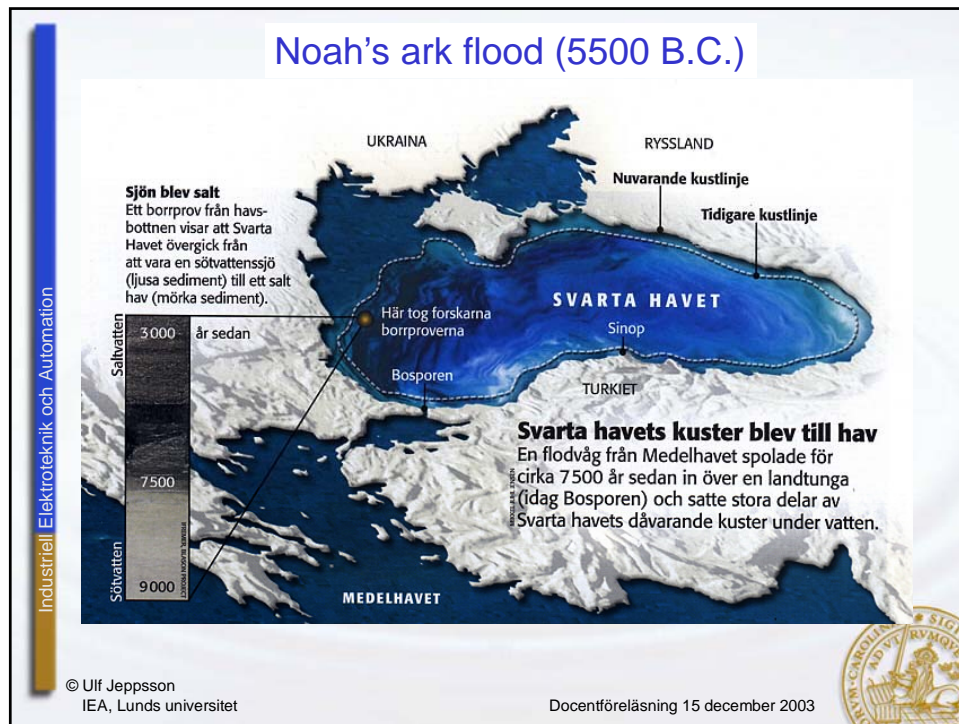
Fresh and salt water

Jeppsson (2003)

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Systems Analysis & Integrated Assessment

= Divide & Conquer

- Integration is a key word → Generalization
- Reflections…

$$\iiint (Watermatex\,2004 + PVR)\,dr\,ds\,dt$$

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Outline

- IWRM : Integrated Water Resources Management
- Within-fence modelling (complete WWTP)
- Ecological Risk Assessment/Management
- Plug&Play modelling
- Distributed Virtual Experimentation
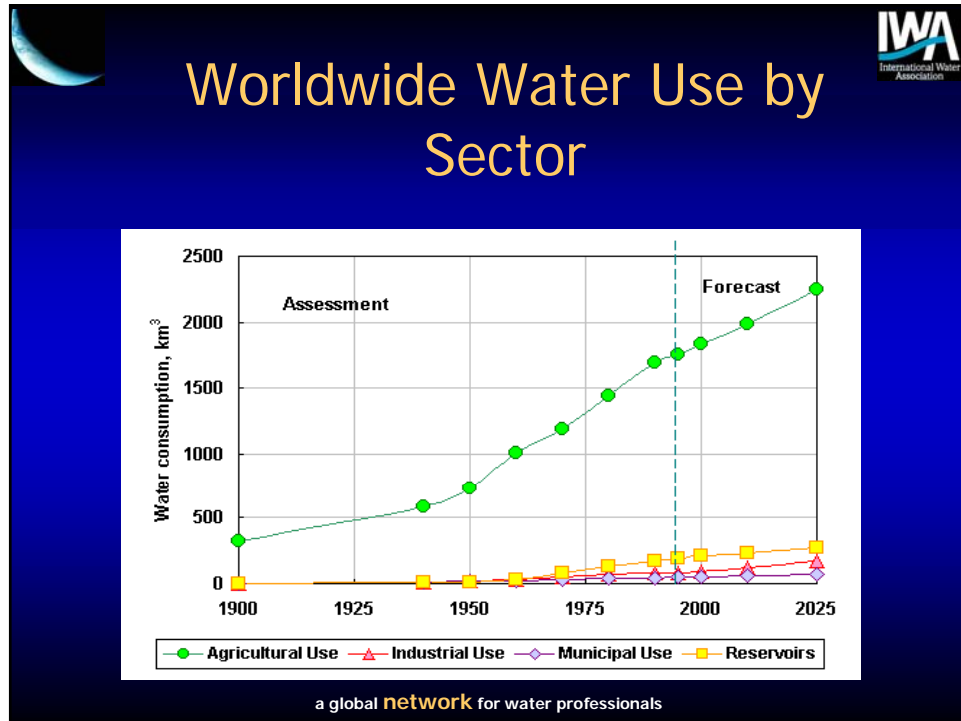- Concluding remarks

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From global to local… (and back)
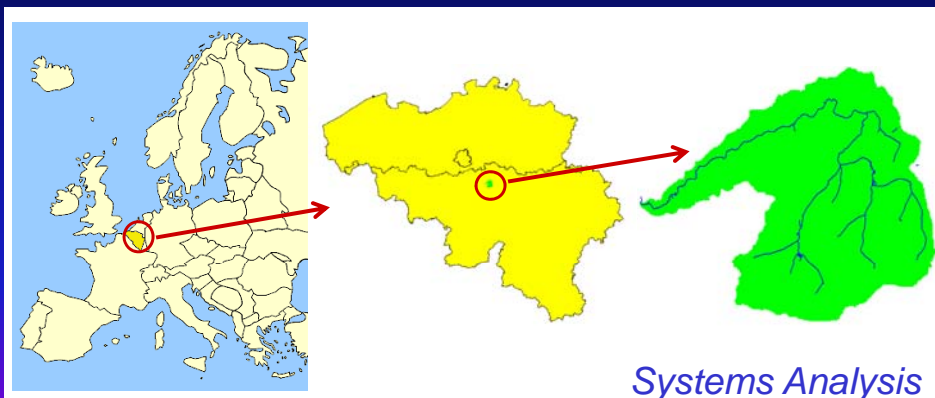
Point sources versus non-point sources

NASA

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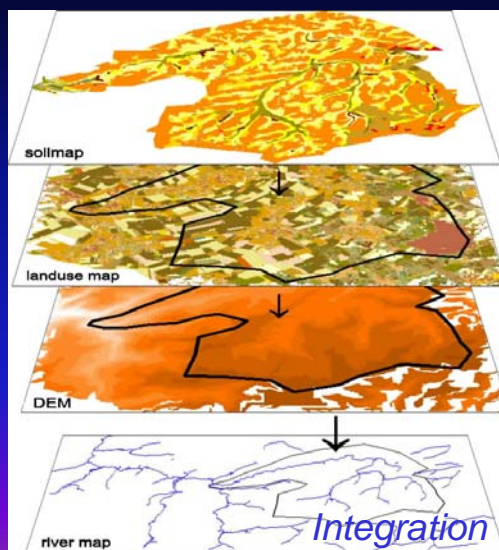
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Diffuse pollution modelling

Nil case study for dynamic pesticide fate modelling

Systems Analysis

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Data collation (GIS-layers)

Integration

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HUMEUR

- HUMEUR = HUMUS for EU (2006 ?)
- HUMUS = Hydrologic Unit Model of the US (1993)

- Nutrients/Pesticides
- Catchment-scale
- Non-point source focus
- SWAT-model (Soil & Water Assessment Tool, USDA)

- HUMUNGOUS™ = HUMUS for the World (????)

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Data collation

- Problematic in Europe
- No common database structure/format
- Different levels of quality/detail
- JRC
  - Joint Research Centre, DG Environment
  - First European database by 2006
  - SWAT-use oriented
  - Uncertainty aspects are considered
  - Information on point pollution is major issue (unexpectedly)

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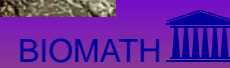- Distributed Virtual Experimentation
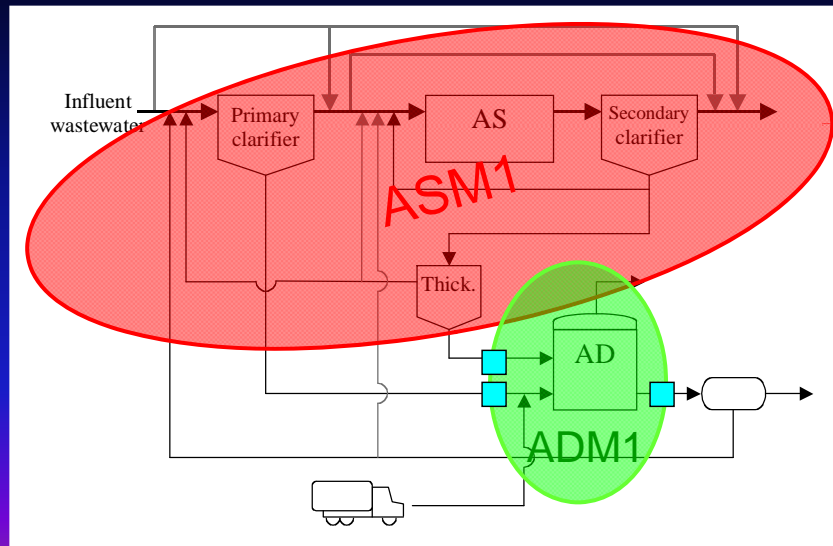- Concluding remarks

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Within-Fence modelling

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Benchmark Simulation Model No. 2

Influent wastewater — Primary clarifier — AS — Secondary clarifier

ASM1

Thick.

AD

ADM1

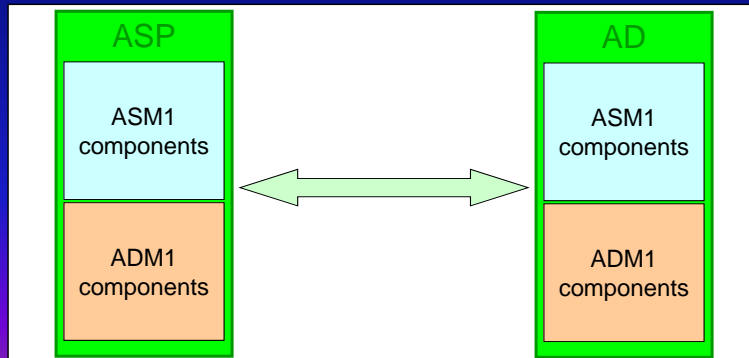Peter A. Vanrolleghem - 17

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Model interfacing

- Principles
  - Elemental balancing (C, H, O, N, P, COD, charge…)
  - System-specific behaviour of components
    must be carefully reflected upon by domain specialists
    (e.g. nitrifiers in waste sludge ending up in digester)
- 3 approaches
  - Supermodel (Dold et al., 2003)
  - One-to-one interfaces (Vanrolleghem et al., 2004)
  - Plant Wide Model Interface (Ayesa et al., 2004)

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Supermodel

- All components are considered in each subsystem
- Behaviour must be described in each subsystem
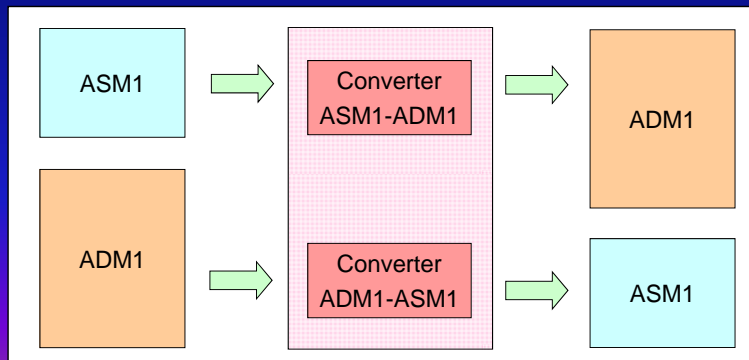- Not scalable when more subsystems are considered

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One-to-one interfaces

- For each model combination, 2 interfaces needed
- $N \times (N-1)/2$ interfaces for N models
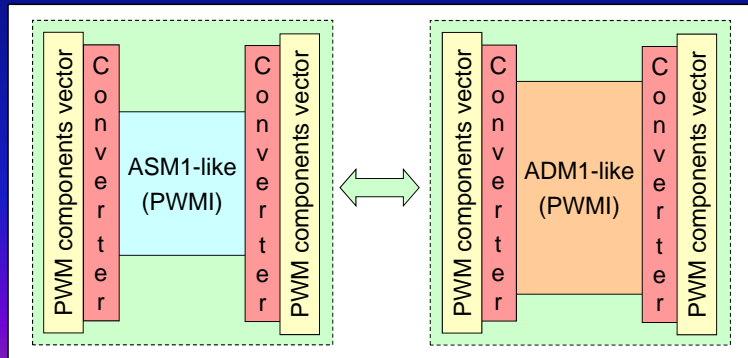- Generalized method to create interfaces is proposed

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Plant-Wide Model Interface

- Bus: models have a "wrapper" to one interface vector
- 2xN interfaces, but if new model: work to be redone
- Generalized method to create interfaces proposed

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Role of SAIA-IWA ?

- Support Benchmarking Task Group
  - Test case for interface development
- Some model upgrading may be useful
  - E.g. pH-modelling in all units
  - Elemental composition in all models
- Time to revise the IWA model suite ? (SBML !)
  - Gernaey et al. (2004): deficiencies in ASM1
  - Gernaey et al. (2004): errors in current reports
- Define IWA standard interfaces
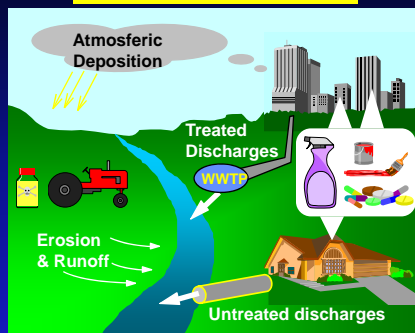 - Agree on underlying assumptions

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Ecological risk assessment

Exposure Analysis

Atmosferic Deposition

Treated Discharges

WWTP

Erosion & Runoff

Untreated discharges

Effects Analysis

Laboratory- and fieldstudies (toxicity tests)

Predicted Environmental Concentration (PEC)
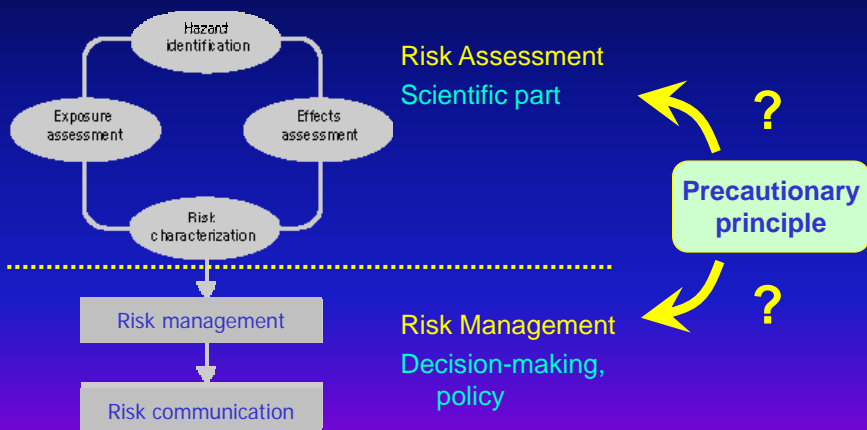
Predicted No Effect Concentration (PNEC)

YES, potential risk

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Ecological risk assessment/management

- Risk analysis of chemical substances:

Risk Assessment
Scientific part

?

Precautionary principle

?

Risk Management
Decision-making, policy

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Include variability & uncertainty

X mg/L

Point estimate

Probabilistic approach

PEC
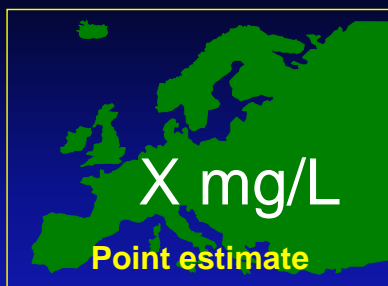
Make more realistic

spatial + temporal + other variability & uncertainty
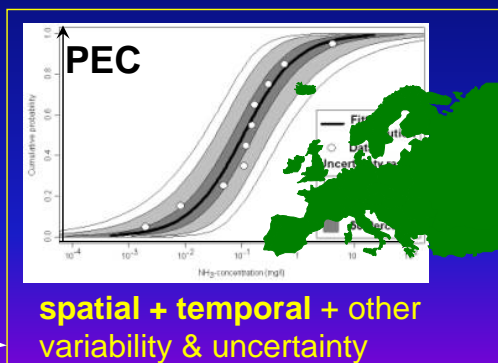
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Reduce spatial variability
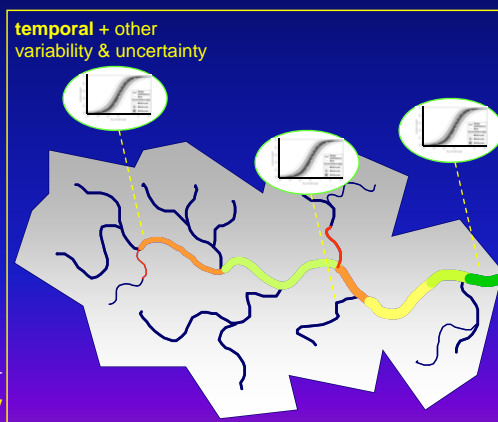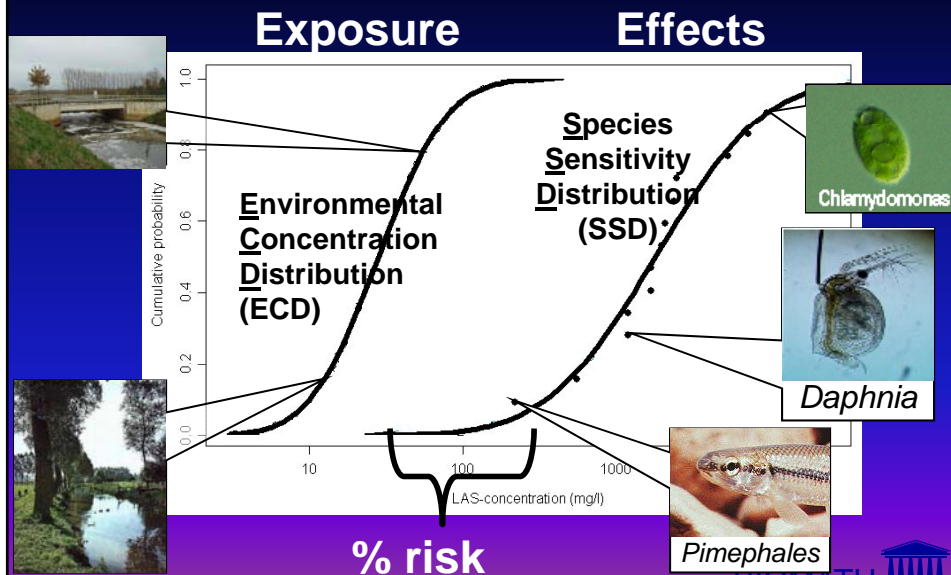
Probabilistic risk assessment

Ecological risk assessment/management

- Detailed information can be made available now
  - Geo-referenced
  - Variability and Uncertainty (Imprecise probabilities)
- How does the manager deal with this ?
  - Summary statistics, indicators
- Where is the divide between
  - Assessment
  - Management
- Where does the precautionary principle belong ?

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Deterministic Risk Assessment

Exposure modelling/ monitoring

Effects assessment

PP   PP

PEC   PNEC

PP

Risk quotient

Risk manageme PP

Verdonck et al.
UPEM conference,
Kollekolle, June 7-9 2004

euras

'Old' EU Deterministic Risk Assessment	Current EU Risk Assessment	Probabilistic Risk Assessment
Exposure modelling/ monitoring — Effects assessment	Exposure modelling/ monitoring — Effects assessment	Exposure modelling/ monitoring — Effects assessment
PP — PP	PP — ECD — SSD	ECD — SSD
PEC — PNEC	PEC — PNEC	
PP	PP	
Risk quotient	Risk quotient	Risk probability + confidence int.
Risk manageme PP	Risk manageme PP	Risk manageme PP

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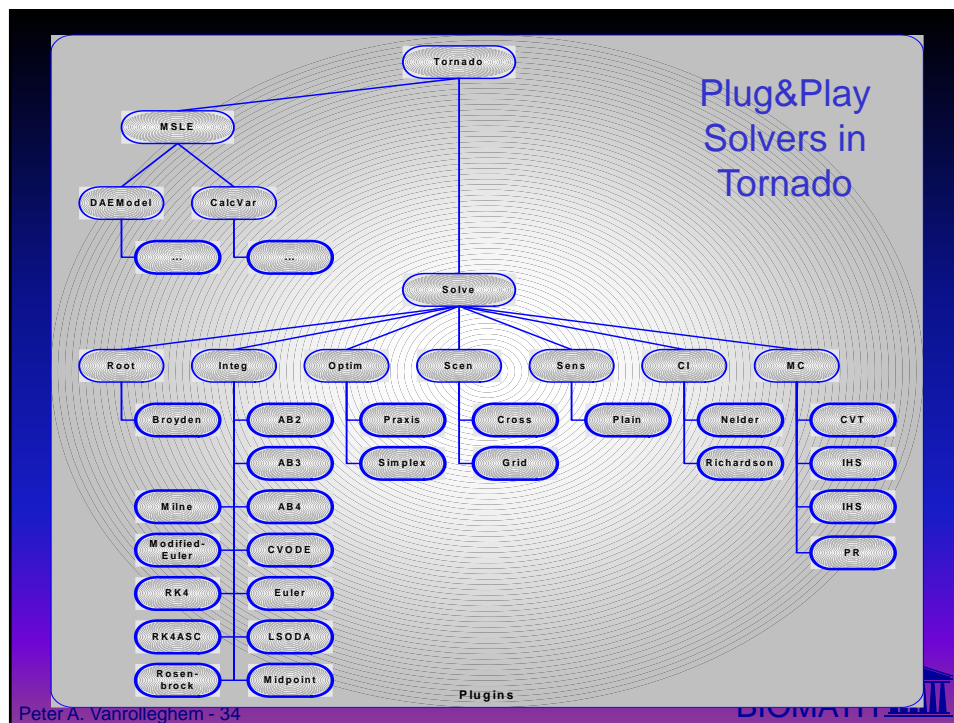- Concluding remarks

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Plug-&-play Modelling

- OpenMI (Blind, Watermatex2004): Software coupling
- Peter Reichert (Watermatex 2004)
  "A standard interface between simulation programs and systems analysis software"
- Pasky Pascual (Beijings News Plaza, 3-4 Nov 04)
  "Modellers shouldn't be coding anymore"
- New back-end of WEST (Tornado)
  software platform
  with defined API
  with plug-&-play capability for tools
  set of available tools
  extensible by "coders"

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Plug&Play
Solvers in
Tornado

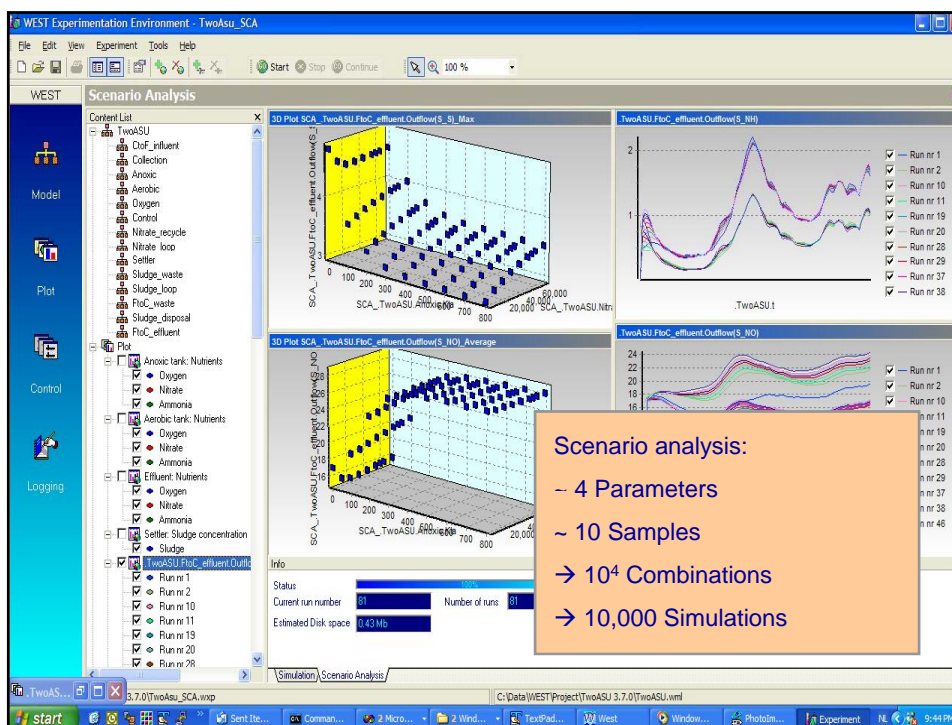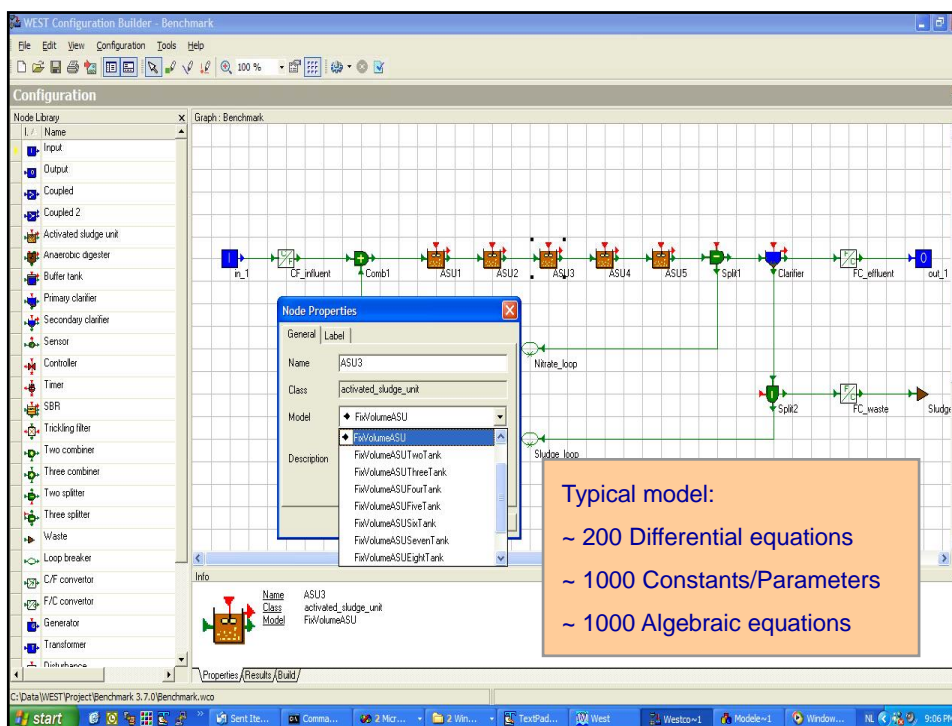Peter A. Vanrolleghem - 34

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Complex virtual experimentation

- Virtual experimentation
  - = model-based studies
  - – For environmental systems: Simulation determines time
- The studies we undertake:
  - – Always take maximum a weekend to calculate…
  - – Become more complex according to Moore's law (x 1.8/yr)
- How to speed up ?

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Typical model:

~ 200 Differential equations

~ 1000 Constants/Parameters

~ 1000 Algebraic equations

Scenario analysis:

~ 4 Parameters

~ 10 Samples

→ 10^4 Combinations

→ 10,000 Simulations

CD4WC project

- <u>C</u>ost-effective <u>d</u>evelopment of urban water systems for <u>W</u>ater Framework Directive <u>c</u>ompliance
  - EU-project
  - Integrated study of sewer-WWTP-river system
  - Methodology for evaluation of design/upgrade scenarios
- Simulations of WWTP options
  - 5 climatic conditions
  - 3 plant sizes (3.000, 30.000, 300.000)
  - 20 options
  - 100 Monte Carlo shots (LHS) for uncertainty propagation

  = 30.000 simulations

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Computational burden in modelling

- Scenario analysis → multiple independent simulations
- Sensitivity analysis → multiple independent simulations
- Monte Carlo analysis → multiple independent simulations
- Optimization :
  - Genetic Algorithm → multiple independent simulations
  - Steepest Descent → multiple dependent simulations
- Experiment Design → multiple independent sensitivity analyses for different parameters

- Robustness Optimization (Walters, Watermatex2004)
  = Optimization of sensitivity analyses
  → multiple independent sensitivity analyses for different parameters
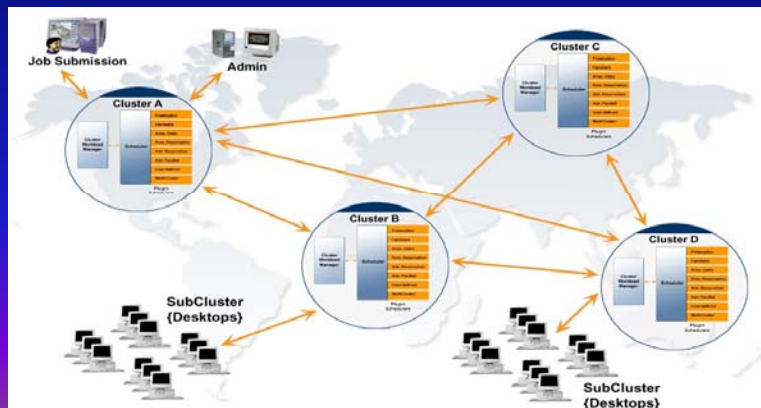
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Distributed Virtual Experimentation

- No split-up of model in submodels that are then simulated over multiple calculation nodes
- Independent virtual experiments (e.g. simulations, sensitivity analyses) can be distributed
- Different approaches to reach this:
  - Grid technology
  - Clustering
  - WDVE (West Distributed Virtual Experimentation)

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Grid technology

- World-wide network of computational & storage nodes
- Virtual organizations

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SuperMUSE Cluster (US EPA, Athens, Georgia)

- Supercomputer for Model Uncertainty and Sensitivity Evaluation
- Babendreier et al. (2002)
- Cluster-based solution
- Linux/Windows mix
- Goal: 384 client PCs, ~1000 GHz
- No other use of PCs possible
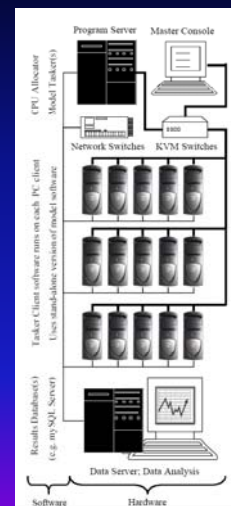
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Idle computers in your offices …

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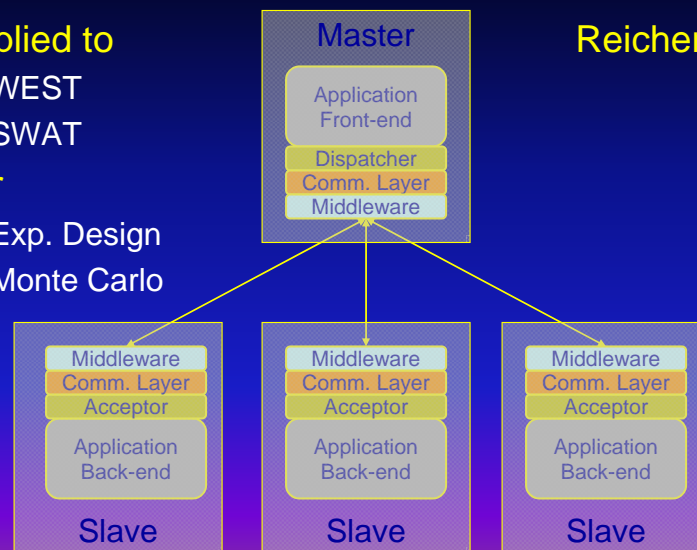
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Distributed Virtual Experimentation

- Applied to
  - WEST
  - SWAT
- For
  - Exp. Design
  - Monte Carlo

Reichert !?

Master

Application Front-end

Dispatcher

Comm. Layer

Middleware

Slave

Middleware

Comm. Layer

Acceptor

Application Back-end

Slave

Middleware

Comm. Layer

Acceptor

Application Back-end

Slave

Middleware

Comm. Layer

Acceptor

Application Back-end

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Take home
(Things to keep you awake ?)

- Characteristics of the Specialist Group on
  Systems Analysis and Integrated Assessment (SAIA)
    - A Generalist Group, not a Specialist Group
    - Galilei : last person to know everything about everything
    - Now: a molecular layer of knowledge above the whole sea
    - Specialist Group: Know everything about something
    - SAIA: Know something about everything

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Take home
(Things to keep you awake ?)

- Possible tasks of Specialist Group on
  Systems Analysis and Integrated Assessment (SAIA)
    - Don't become a "Specialist" group, but "Generalist" group
    - Remain multidomain in interest
    - Support Task Groups (BSM, Calibration guidelines)
    - Direct Task Group on Modelling ASPs
    - Be at the nexus of policy-law-science

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