# The Multi-Run Simulation Environment SimEnv

## or: Would you trust an orthopaedist who never x-rays?

http://www.pik-potsdam.de/software/simenv


| | |
|---|---|
| **Michael Flechsig** | **PIK – Potsdam Institute for Climate Impact Research, Potsdam, Germany** |
| **Uwe Böhm** | **DWD – German National Meteorological Service** |
| **Thomas Nocke** | **PIK** |
| **Claus Rachimow** | **PIK** |

# SimEnv is . . .

- a multi-run simulation environment
- that addresses the evaluation and usage of simulation models
- mainly for uncertainty, sensitivity and scenario analyses
- applying pre-formed probabilistic, deterministic and Bayesian sampling strategies
- in high-dimensional (100+) parameter / initial value spaces of simulation models
- with large volume (GB) of multi-variate (100+) and multi-dimensional (≤9) model output

# Motivation: Global Change Research

- Model development and application as key working techniques
- Complexity of the Earth system, intrinsic variability of processes, limits of knowledge
- Growing demand for uncertainty and sensitivity measures in Earth system models
- Need for communicating uncertainty to the community, stakeholders and the public

Nature, 486, 183-184 (2012)

**Climate models at their limit?**

Estimates of climate-change impacts will get less, rather than more, certain. But this should not excuse inaction, say **Mark Maslin and Patrick Austin**.

Nature Climate Change, 3, 769-771 (2013)

**Uncertainty analysis in climate change assessments**

Richard W. Katz, Peter F. Craigmile, Peter Guttorp, Murali Haran, Bruno Sansó and Michael L. Stein

Use of state-of-the-art statistical methods could substantially improve the quantification of uncertainty in assessments of climate change.

Nature Climate Change, 1, 198-200 (2011)

**Opportunities from uncertaintie[s]**

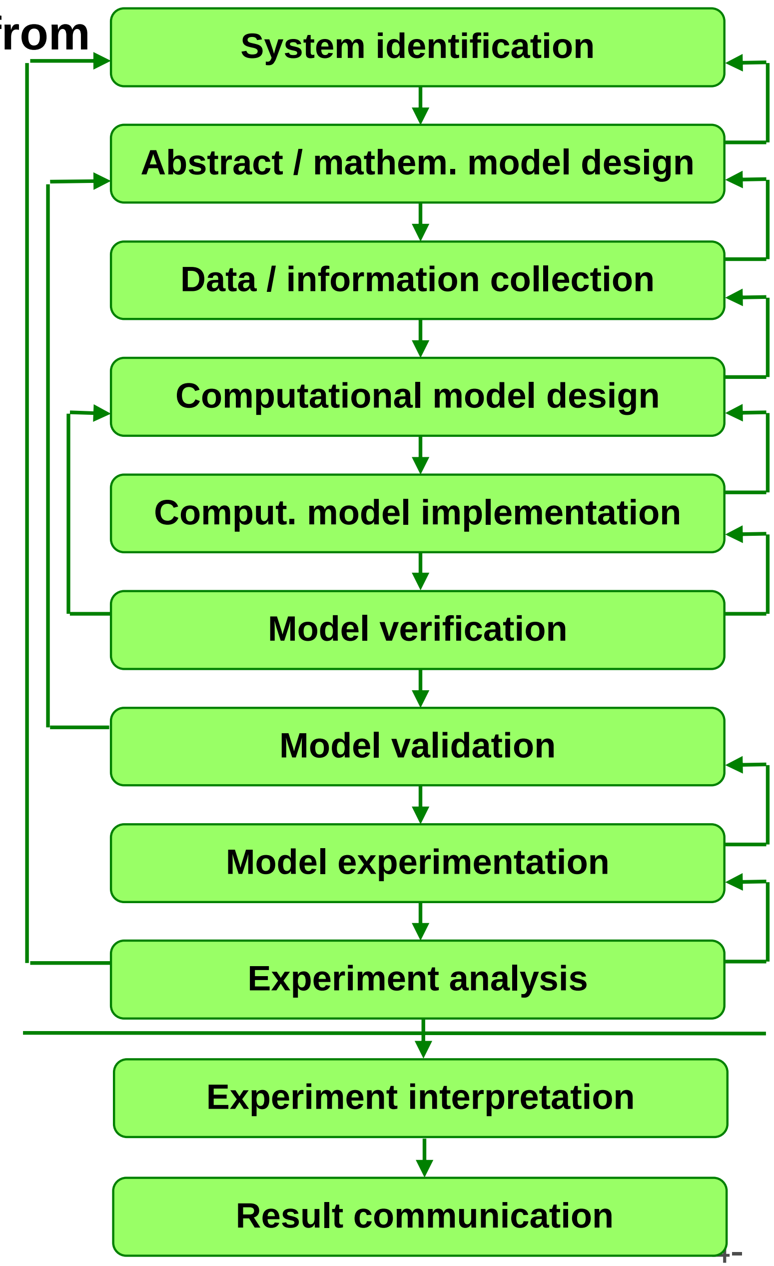
The inability to verify nations' reported progress towards emission-reduction commitments is a stumbling block in climate change negotiations. Narrowing uncertainties in the global carbon cycle could help overcome this obstacle.

Gary W. Yohe

# Model Uncertainties

**Uncertainties in modelling and experimentation arise from**

- Framing / delimitation of the modelled system's part
- Inherent properties of the real system
- Incomplete knowledge about the real system
- Mathematical model
- Model implementation
  (discretization schemes, numerical algorithms, …)
- Model parametrization and parameter variability
- Machine accuracy (rounding errors, …)
- Experiment settings (scenarios, drivers)
- Multi-model variability (e.g., CMIPs, ISI-MIP)
- Interpretation of model results
- Communication of experiment findings



# Sensitivity & Uncertainty Analyses

**Sensitivity Analysis SA** (A. Saltelli, JRC Ispra)

The study of how the uncertainty in the model output / states can be apportioned to different sources of uncertainty in the model input

**Uncertainty Analysis UA** (P. Janssen, RIVM)

The study of the uncertain aspects of a model and of their influence on the (uncertainty of the) model output / states

- SA is more straightforward: it is on uncertainty decomposition
  UA is more general: it is on uncertainty propagation & quantification

- Consider

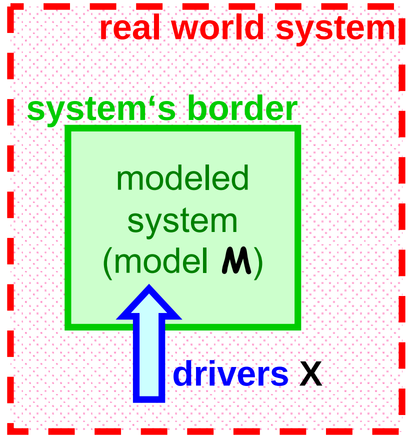
$$\mathbf{M}: \quad \{Z_t\} = F(\{Z_{t-\Delta t}\}, \{Z_0\}, \{P\}, \{X_t\}), \quad \{Y_t\} = f(\{Z_t\}) \quad \text{(example)}$$

as

$$\mathbf{M}: \quad Y = g(\mathbf{x}) \qquad \mathbf{x} = (x_1, x_2, \ldots, x_k) \subset \{P, Z_0\}$$

$= k$ **input factors**: subset of parameters $\{P\}$ and initial values $\{Z_0\}$

$Y$ = model output / states $Z$



# Model vs. SA Method Characteristics

## Models

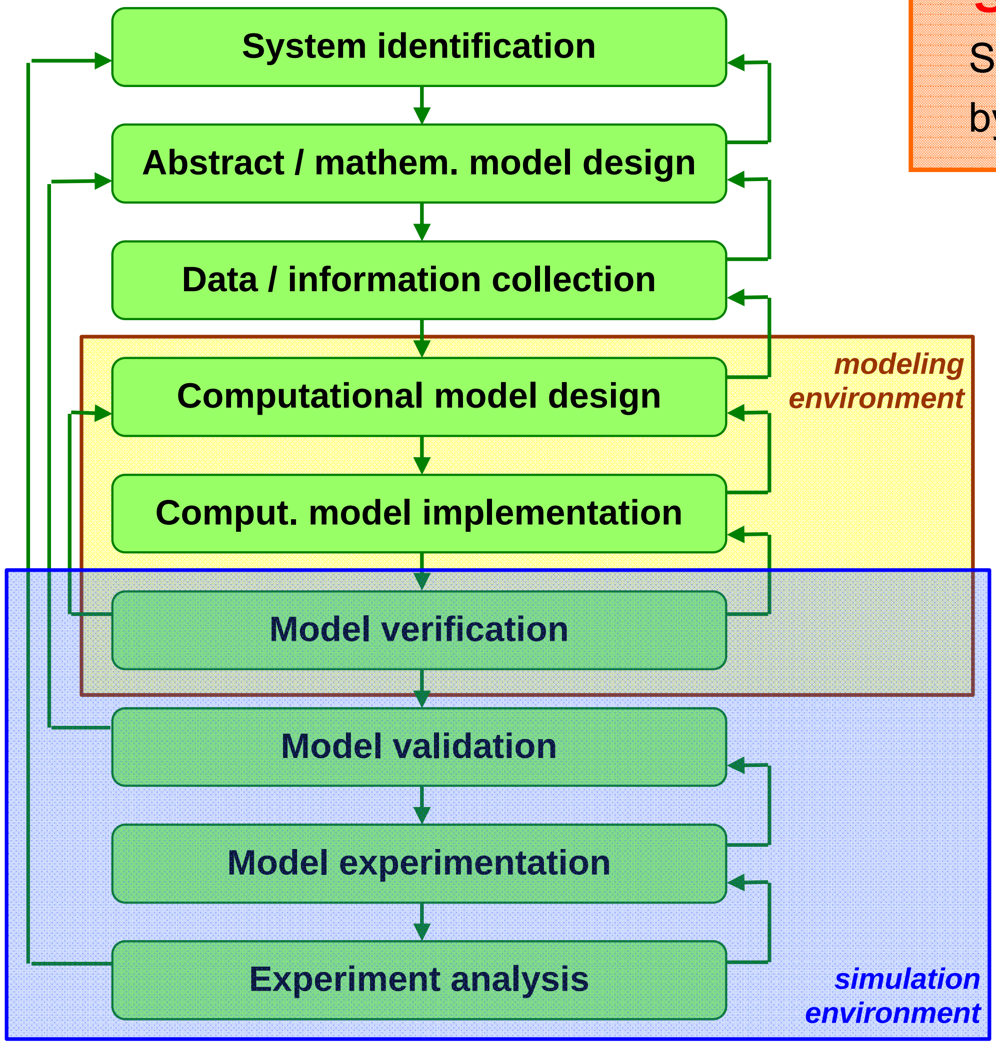
- **(M1)** Complex phenomena (nonlinear, threshold effects, strong interactions)
- **(M2)** Large number of uncertain factors
- **(M3)** High computational costs (often) in terms of CPU time consumption
- **(M4)** Large volume of multi-dimensional model output of interest

## SA Methods (A. Saltelli)

- **(M1)** → Model independency → **model free**
  - Applicable to non-linear / non-additive / non-monotonic models
- **(M1)** → Factor variability
  - Consider the whole range of factor variation e.g., by a pdf
- **(M1)** → Multi-factor measures
  - Simultaneously take into account variation of all factors

  (Factor variability and multi-factor measures) → **global method**
- **(M2)** → Factor grouping
  - Treat grouped factors as if they were single factors
- **(M3)** → Cost efficiency → **computational costs C**
  - In terms of the number of single simulation runs

# Simulation Environments




**Simulation environment** =
Software tool to support experimenting with models by a structured approach

Model $\boldsymbol{M}$: $y = f(\mathbf{x})$

- Typical questions (settings)
  - How does a factor x influence y?
  - What are the most sensitive factors on y?
  - What is the factor value that minimizes y?
- Experiment steps to answer a question about $\boldsymbol{M}$
  - Design
  - Perform
  - Analyze

# Requirements for Simul. Environments

- Open architecture
  - Model interface
  - Import sampled factor values into model (*)
  - Export model output directly from the model to the environment or
    transform at least native model output to data structures of the simulation environment

- Load distribution (*)
  - Parallelize the experiment
    if sample can be drawn before the experiment

- Experiment analysis
  - (i) Single run related aggregation and transformation operators
    for the model state space
    (ii) Method-specific operators to derive measures
    over the run ensemble / at the experiment factor space (*)
  - Apply explorative visualization techniques to experiment output and measures

- Data interface
  - Import reference data into simulation environment
  - Export data from experiment analysis

(*) = for multi-run environments

# SimEnv: The Basics

- Focus on sample-based experiment techniques
  for uncertainty, sensitivity and scenario analyses

- Support of high-dimensional factor spaces and
  models with large volume of multi-variate / multi-dimensional output

- Simple model interface for factors and model output

  **“include for each factor and for each model output field
  one SimEnv function call into model source code”**

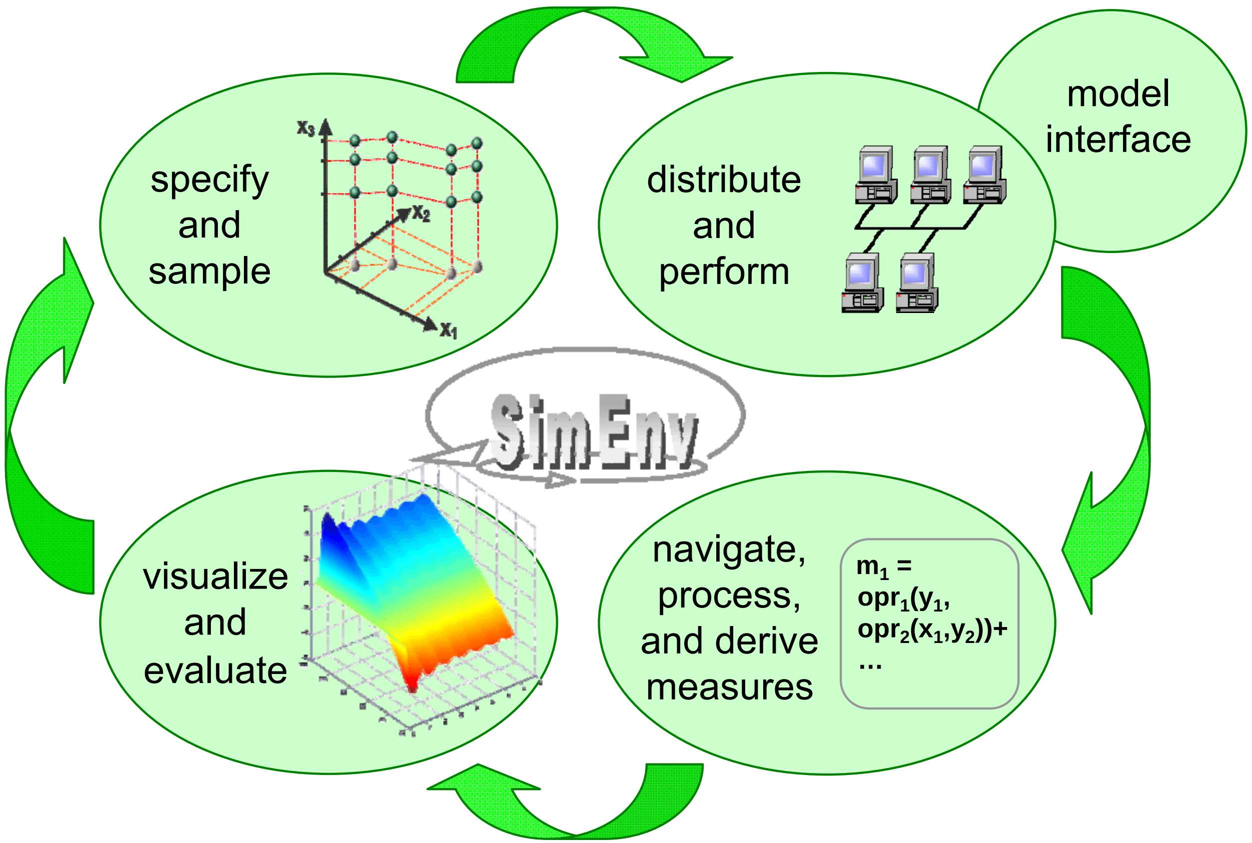
  | | | | | |
  |---|---|---|---|---|
  | at programming language level: | C/C++ | Fortran | Java | Python |
  | at modeling / tool language level: | Matlab | Mathematica | GAMS | R (in prep.) |
  | at shell script level and for native model ASCII file output | | | | |

- Storage of model output of such interfaced models and of analysis results in
  self-describing NetCDF or IEEE compliant binary format

- Distribution of the single runs of an experiment
  at a compute cluster (using MPI) or at a multi-core machine

- Interactive experiment postprocessor with 100+ operators and coupled visualization framework
  SimEnvVis

# Basic SimEnv Workflows



# SimEnv Built-in Experiment Types

| Experiment type | glo-bal | model-free | corre-lated factors | computational costs (k factors) |
|---|---|---|---|---|
| Qualitative Factor Ranking (Morris method) | ✓ | ✓ | | $C \approx 10*(k+1)$ |
| Variance Decomposition (Sobol' method) | ✓ | ✓ | | $C = N_{MC}*(k+2)$ |
| Monte Carlo Analysis | ✓ | ✓ | ✓ | $C = N_{MC}$ |
| Local Sensitivity Analysis (linearity, symmetry …) | | ✓ | | $C = 2*k$ |
| Deterministic Factorial Design (OAT, full/fractional) | (✓) | ✓ | ✓ | C= |
| Bayesian Calibration (Metropolis algorithm) | ✓ | ✓ | ✓ | $C \gg N_{MC}$ |
| Optimization (simulated annealing) | ✓ | ✓ | (✓) | C = |

# Example: Model Interface

**model source code**

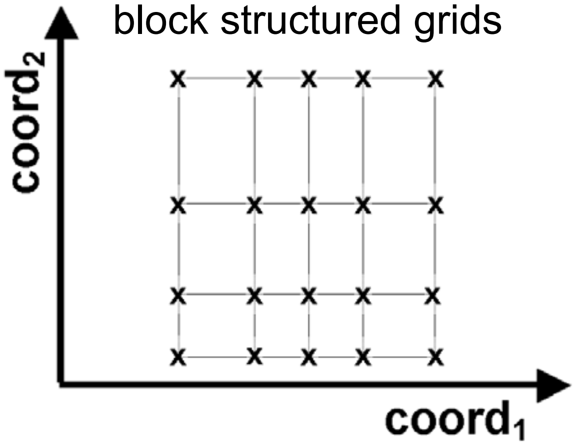
```
…
real*8 y(180,360,100)
x1 = 5.

x2 = 4.

… (compute model output y)
istatus = simenv_put_f('y',y)
…
```

**SimEnv model output description**

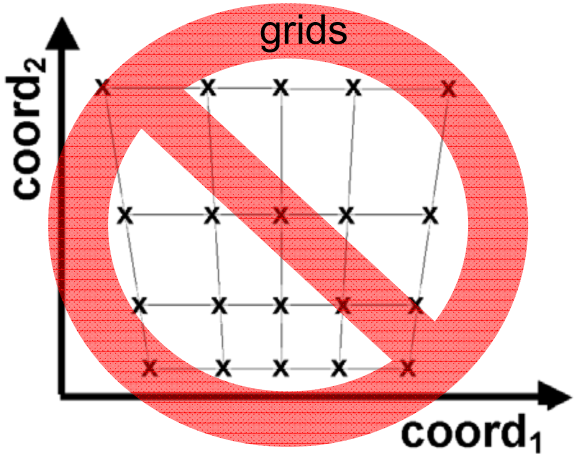
| | | | |
|---|---|---|---|
| coordinate | lat | descr | geographic latitude |
| coordinate | lat | values | equidist_end 89.5 (-1) -89.5 |
| coordinate | lon | values | equidist_nmb -179.5 (1) 360 |
| coordinate | time | values | list 1,2,3, …, 98,99,100 |
| variable | y | descr | … |
| variable | y | type | real*8 |
| variable | y | coords | lat , lon , time |
| variable | y | index_ext | 1:180 , 1:360 , 1:100 |

**generate grid**

variables on rectilinear / block structured grids




variables on curvilinear grids



# Example: Model Interface

***Modified model source code***

```
…
real*8 y(180,360,100)
x1 = 5.

x2 = 4.

… (compute model output y)
istatus = simenv_put_f('y',y)
…
```

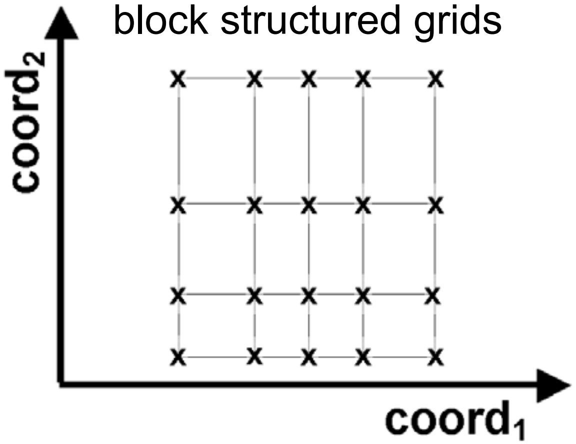
***SimEnv model output description***

| | | | |
|---|---|---|---|
| coordinate | lat | descr | geographic latitude |
| coordinate | lat | values | equidist_end 89.5 (-1) -89.5 |
| coordinate | lon | values | equidist_nmb -179.5 (1) 360 |
| coordinate | time | values | list 1,2,3, …, 98,99,100 |
| variable | y | descr | … |
| variable | y | type | real*8 |
| variable | y | coords | lat , lon , time |
| variable | y | index_ext | 1:180 , 1:360 , 1:100 |

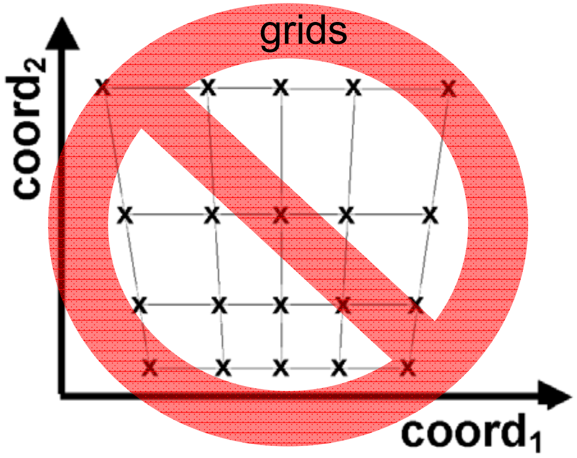
blue line + green line :
associate
SimEnv model output
description variable y
with
model source code variable y
and
output real*8 field y

**generate grid**

variables on rectilinear / block structured grids




variables on curvilinear grids



# Example 1: Experiment Description

### *Modified model source code*

```
…
real*8 y(180,360,100)
x1 = 5.
istatus = simenv_get_f('x1',x1,x1)
x2 = 4.
istatus = simenv_get_f('x2',x2,x2)
… (compute model output y)
istatus = simenv_put_f('y',y)
…
```

### *SimEnv model output description*

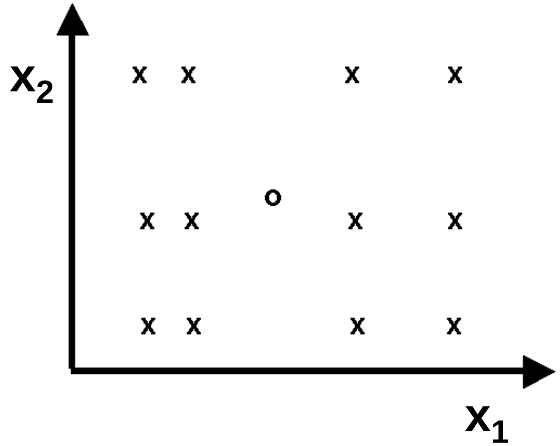
| | | | |
|---|---|---|---|
| coordinate | lat | descr | geographic latitude |
| coordinate | lat | values | equidist_end 89.5 (-1) -89.5 |
| coordinate | lon | values | equidist_nmb -179.5 (1) 360 |
| coordinate | time | values | list 1,2,3, … ,98,99,100 |
| variable | y | descr | … |
| variable | y | type | real*8 |
| variable | y | coords | lat , lon , time |
| variable | y | index_ext | 1:180 , 1:360 , 1:100 |

DFD = Deterministic Factorial Design

### *SimEnv experiment description*

| | | | |
|---|---|---|---|
| general | | type | DFD |
| factor | x1 | default | 5 |
| factor | x1 | sample | list 2, 3, 7, 10 |
| factor | x2 | default | 4 |
| factor | x2 | sample | list 1, 3.5, 7 |
| specific | | comb | x1*x2 |

**generate sample**



# Example 1: Experiment Description

***Modified model source code***

```
…
real*8 y(180,360,100)
x1 = 5.
istatus = simenv_get_f('x1',x1,x1)
x2 = 4.
istatus = simenv_get_f('x2',x2,x2)
…  (compute model output y)
istatus = simenv_put_f('y',y)
…
```

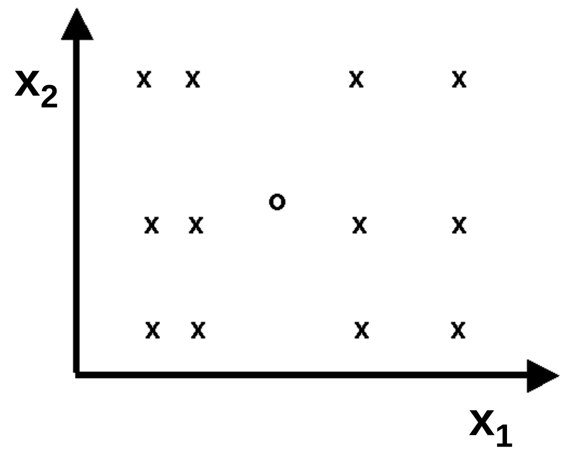
***SimEnv experiment description***

| | | | |
|---|---|---|---|
| general | | type | DFD |
| factor | x1 | default | 5 |
| factor | x1 | sample | list 2, 3, 7, 10 |
| factor | x2 | default | 4 |
| factor | x2 | sample | list 1, 3.5, 7 |
| specific | | comb | x1*x2 |

(green line): associate SimEnv experiment description factor $x_1$ with model source code parameter $x_1$

(blue line): get adjusted model source code parameter

**generate sample**



# Example 2: Monte Carlo Analysis

***Modified model source code***

```
…
real*8 y(180,360,100)
x1 = 5.
istatus = simenv_get_f('x1',x1,x1)
x2 = 4.
istatus = simenv_get_f('x2',x2,x2)
…  (compute model output y)
istatus = simenv_put_f('y',y)
…
```

***SimEnv model output description***

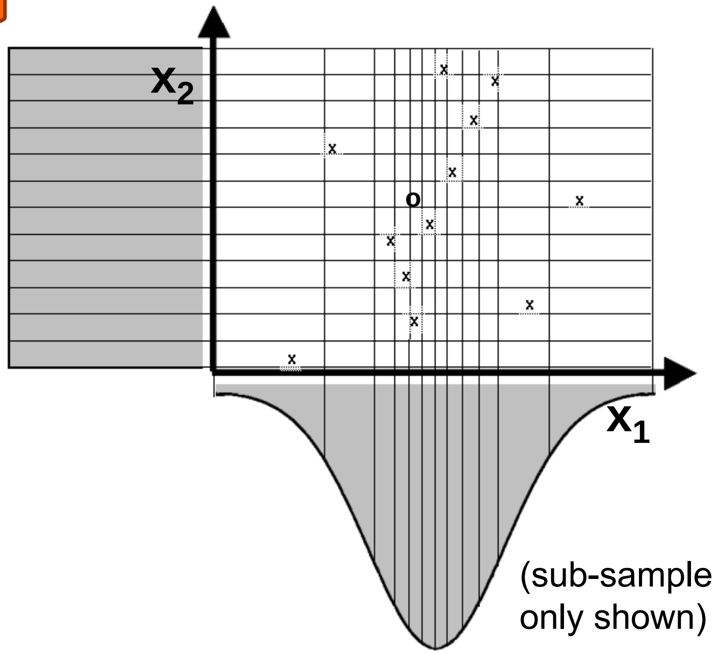
| | | | |
|---|---|---|---|
| coordinate | lat | descr | geographic latitude |
| coordinate | lat | values | equidist_end 89.5 (-1) -89.5 |
| coordinate | lon | values | equidist_nmb -179.5 (1) 360 |
| coordinate | time | values | list 1,2,3, … ,98,99,100 |
| variable | y | descr | … |
| variable | y | type | real*8 |
| variable | y | coords | lat , lon , time |
| variable | y | index_ext | 1:180 , 1:360 , 1:100 |

UNC_MC = Monte Carlo Analysis

***SimEnv experiment description***

| | | | |
|---|---|---|---|
| general | | type | UNC_MC |
| factor | x1 | default | 5. |
| factor | x1 | sample | distr N(5.,0.5) |
| factor | x1 | s_method | stratified |
| factor | x2 | default | 4. |
| factor | x2 | sample | distr U(3.5,4.5) |
| factor | x2 | s_method | stratified |
| specific | | runs | 250 |

**generate sample**



# Experiment Description File

- To generate a sample in the factor space under study
  an experiment type has to be equipped with numerical information

| | | | | |
|---|---|---|---|---|
| general | | type | UNC_MC | # (**M**) experiment type Monte Carlo Analysis |
| factor | x1 | descr | parameter influencing … | # description |
| factor | x1 | unit | kg/m**2 | # unit |
| factor | x1 | default | 1. | # (**M**) factor nominal value |
| factor | x1 | type | add | # (**M**) add sampled values to nominal value |
| factor | x1 | sample | distr N(1,0.04) | # (**M**+**E**) X1 ~ N(1,0.04) normal distribution |
| factor | x1 | sample_method | pseudo | # use "standard" random number generator |
| factor | x1 | sample_include | 0.4:1.6 | # sample only within 3σ interval |
| factor | x2 | … | | |
| factor | x2 | sample | distr U(-5,5) | # X2 ~ U(-5,5) uniform distribution |
| factor | x2 | sample_method | stratified | # use Latin hypercube sampling |
| factor | x3 | … | | |
| factor | x3 | sample | file MyOwnSample.dat | # import sample for X3 from file |
| specific | | runs | 5000 | # (**M**+**E**) max. number of Monte Carlo runs |
| specific | | function | sum(sin(y+3*x1)-avg(y)) | # model output function for optional UNC_MC stopping rule |

**M** = mandatory
**E** = experiment type specific

# Experiment Analysis

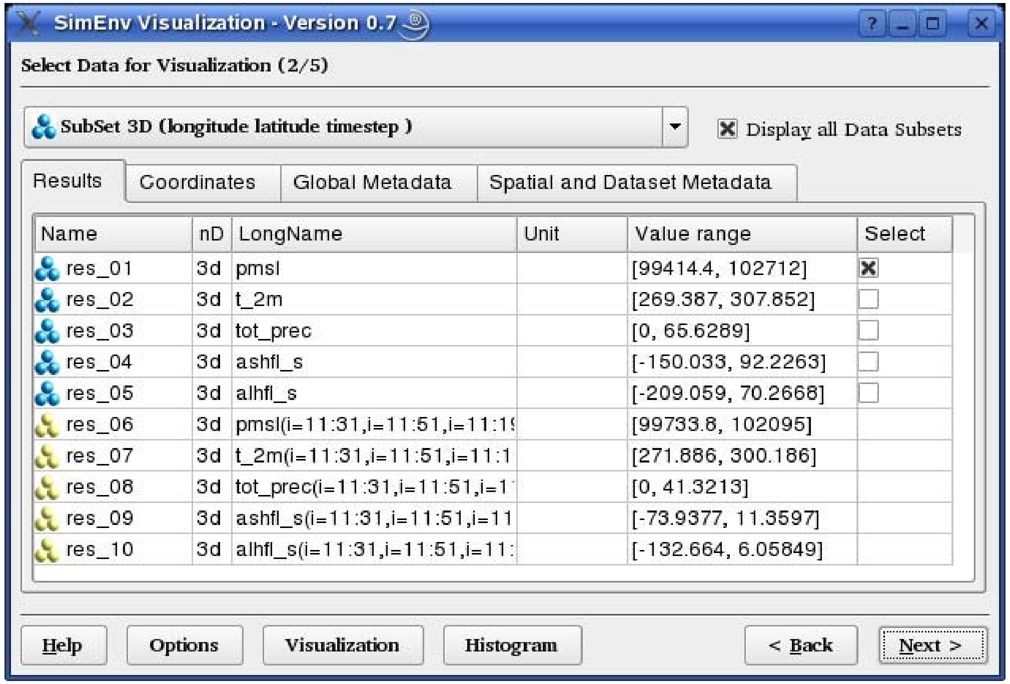
- Process (aggregate, transform, …) experiment output and derive measures

- By navigating the model output (state variable) space {y}
  and the experiment (factor) space $\{X_k\}$

- Compute secondary output from model output and
  derive experiment related measures over $\{X_k\}$
  by application of operator chains
  to experiment output, reference data and other SimEnv experiments
  - > 100 built-in operators
  - Interface to plug in user-defined operators

- Visual experiment analysis and evaluation
  by the visualization framework SimEnvVis

# SimEnvVis Visualization Framework



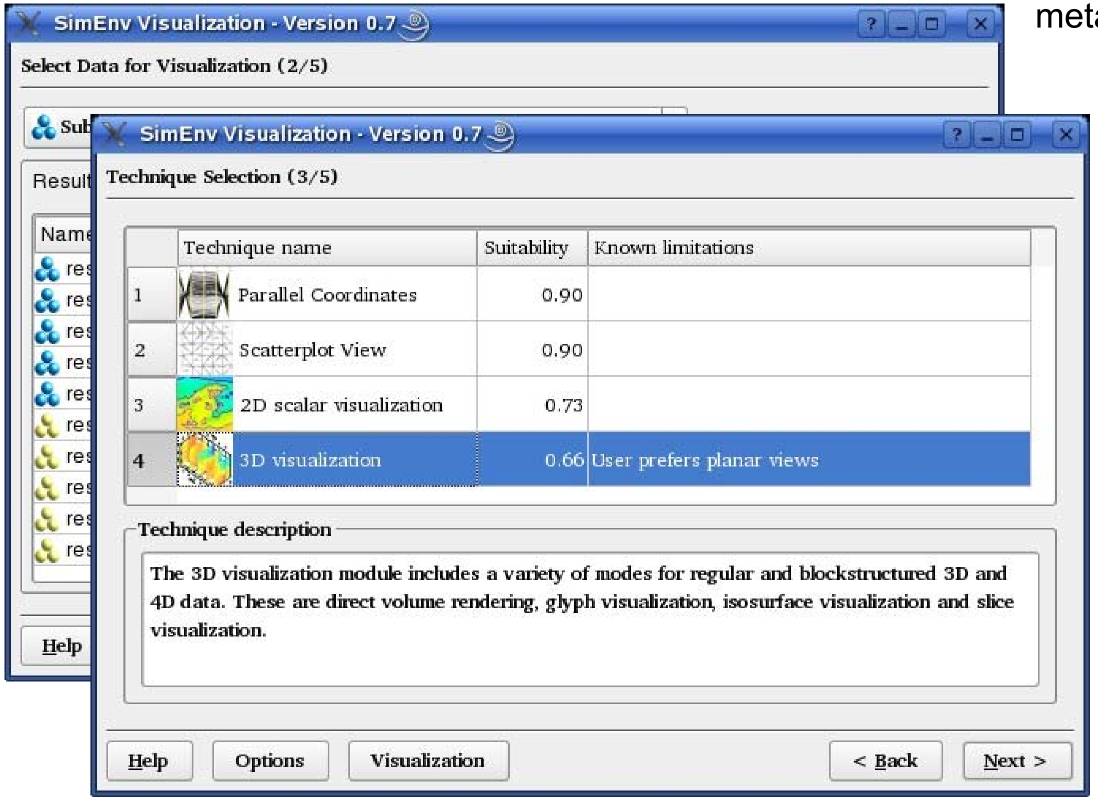

metadata display, adaptation, filtering

**SimEnvVis** (T. Nocke, PIK and M. Heitzler, ETH Zurich):

A visualization framework consisting of

- a wizard to analyze data, select a technique and parametrize it and
- coupled visualization systems / maps

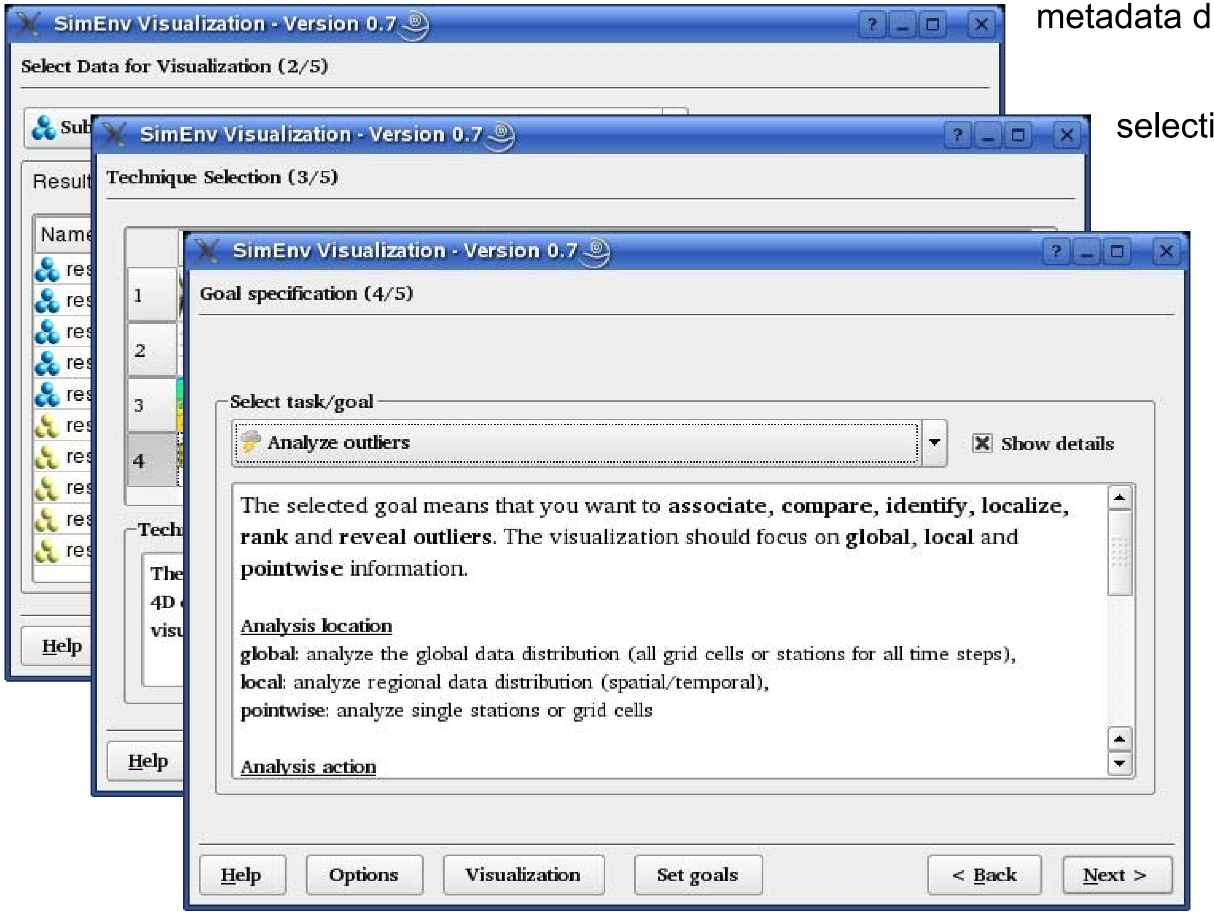
# SimEnvVis Visualization Framework




metadata display, adaptation, filtering

selection of suited visualization techniques

# SimEnvVis Visualization Framework

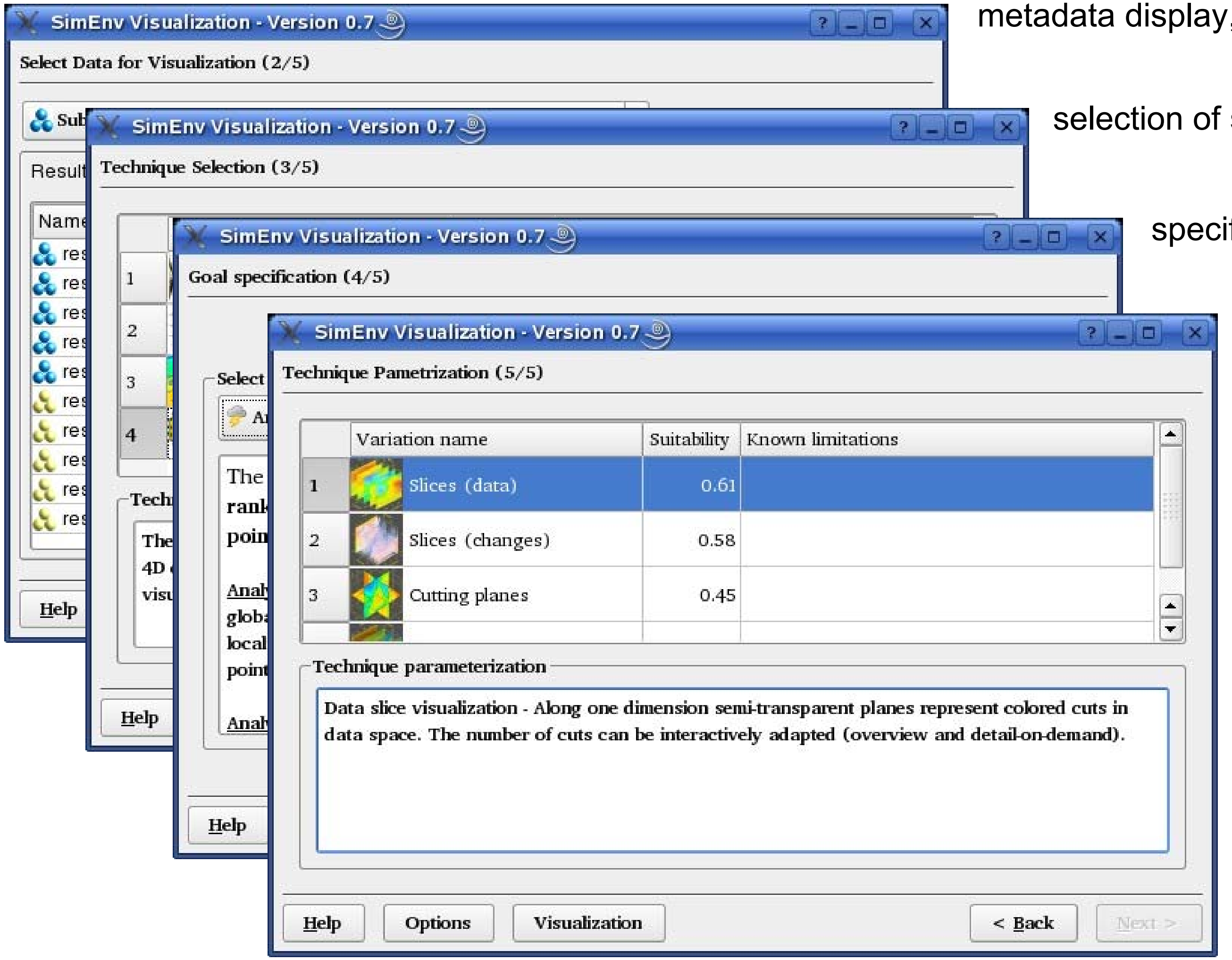



metadata display, adaptation, filtering

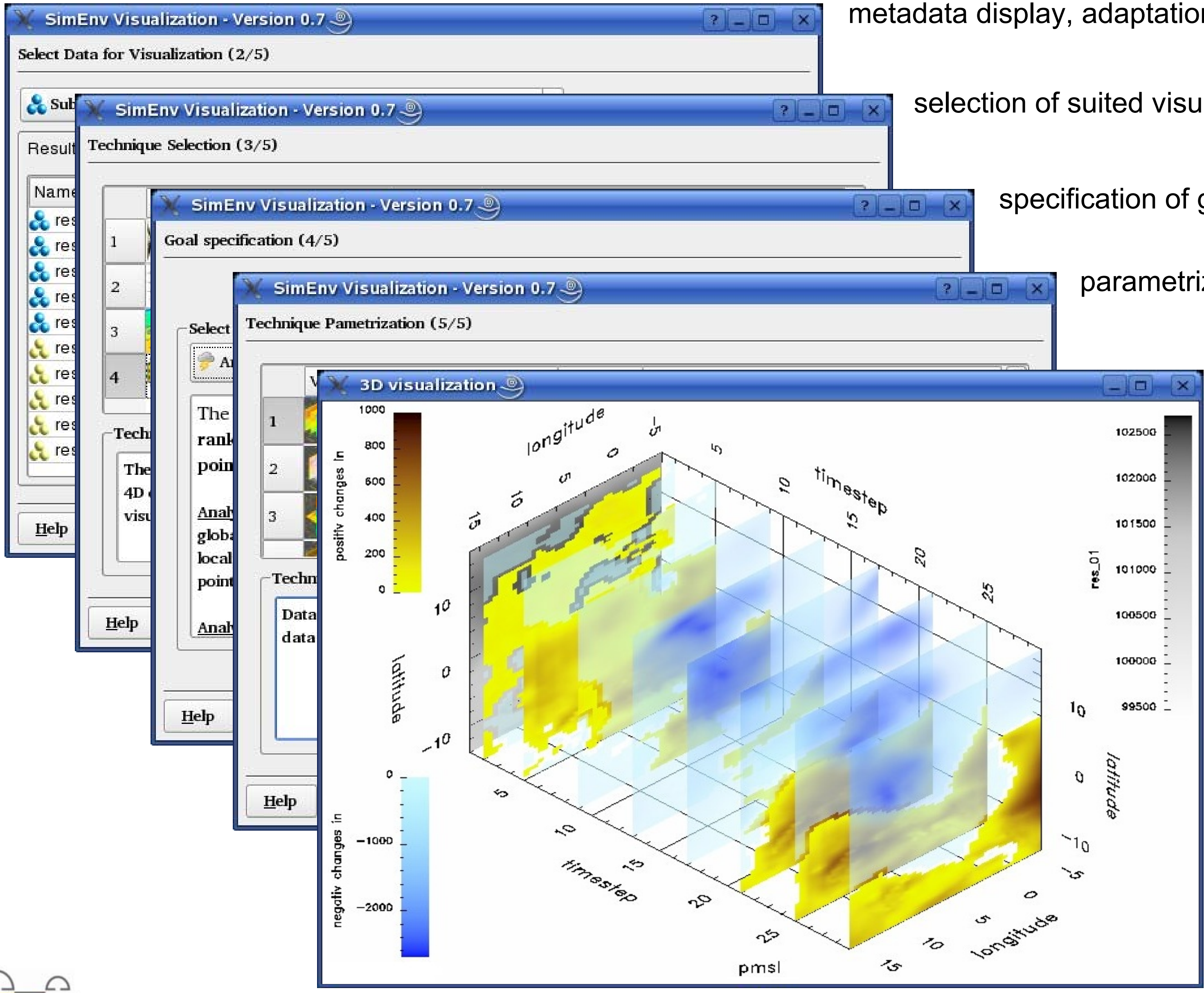
selection of suited visualization techniques

specification of goals

# SimEnvVis Visualization Framework



# SimEnvVis Visualization Framework




metadata display, adaptation, filtering

selection of suited visualization techniques

specification of goals

parametrization

start of interactive visualization

**regional climate model CCLM**

# Some SimEnv Applications at PIK

| | Model | SimEnv Application | Model Interface |
|---|---|---|---|
| PIK | **4C** | regional model applications, factorial designs, Bayesian calibration | Fortran |
| PIK | **Aeolus** | parameter sensitivity of the cloud module | C++ |
| PIK | **Climber-2** | parameter screening / sensitivity, MCA, comparison of multi-parameter settings | Fortran |
| PIK | **CLM** | parameter screening | script level, Fortran |
| PIK | **LPJmL** | global / regional model application, parameter sensitivity | Fortran, C, script level |
| PIK | **MICA** | parameter screening for stabilization of climate coalitions games | GAMS |
| PIK | **Monsoon** | global sensitivity, uncertainty | Fortran, C, script level |
| PIK | **REMIND** | parameter screening uncertainty analyses | GAMS |
| outside PIK | **Lagom** | model inspection, global sensitiv. analyses, initial value and parameter sensitivity | Java / Scala, Matlab, Mathematica |
| outside PIK | **Island** | model sensitivity: Monte Carlo, Morris method, variance decomposition | GAMS |

# SimEnv Usage Statistics (PIK, 10 yrs.)

- Total

| | sum | ~ per day |
|---|---|---|
| Users | 40+ | |
| Models | 30+ | |
| Services | 65.000 | 18 |
| Experiments | 15.000 | 4 |
| Single runs | 4.000.000 | 1.100 |
| Post-processor sessions | 28.000 | 8 |

Experiment types
67% Deterministic factorial design
19% Monte Carlo analysis
5% Factor ranking / Morris
9% other types

- Per experiment

| | min | mean | max |
|---|---|---|---|
| Single runs | 2 | 288 | 50.000 |
| Factors | 1 | 8 | 50 |
| Output variables | 1 | 11 | 97 |
| Output values / single run | 1 | $50*10^3$ | $30*10^6$ |
| Output bytes / single run | 4 | $205*10^3$ | $125*10^6$ |
| Output bytes / experiment | 40 | $51*10^6$ | $18*10^9$ |
| Used processor cores | 3 | 56 | 255 |

# Summary / Conclusions

**SimEnv ...**

- ... is an experimentation tool to cope with model sensitivity and uncertainty by multi-run simulations from different perspectives
- ... enables a quick and easy approach for standard tasks of simulation models' quality assurance
- ... copes with high-dimensional factor spaces and large volume multi-dimensional model output
- ... supplies simple model and operator interfaces
- ... easily generates NetCDF model and post-processor output
- ... incorporates high-end visual evaluation of post-processed experiment output

# Further Reading

## Sensitivity & uncertainty analyses


- Eykhoff, P. (1974) System identification: Parameter and state estimation. John Wiley & Sons
- Sobol', I.M. (1993) Sensitivity estimates for non-linear mathematical models. Math. Model. Comput. Exp., 1, 407-414
- McKay, D.J. (2004) Information theory, inference, and learning algorithms. Cambridge
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## SimEnv and applications


- Flechsig, M., Böhm, U., Nocke, T., Rachimow, C. (2005): Techniques for quality assurance of models in a multi-run simulation environment. In: Hanson, K.M. and Hemez, F.M. (eds.): Sensitivity Analysis of Model Output. Los Alamos National Laboratory, Los Alamos, NM, USA, 297-306
- Böhm, U., Kücken, M., Hauffe, D., Gerstengrabe, F.-W., Werner, P.C., Flechsig, M., Keuler, K., Block, A., Ahrens, W., Nocke, T. (2004): Reliability of regional climate model simulations of extremes and of long-term climatic characteristics. Natural Hazards and Earth System Sciences (NHESS), 4: 417 – 431
- Knopf, B., Flechsig, M., Zickfeld, K. (2006): Multi-parameter uncertainty analysis of a bifurcation point. Nonlin. Processes Geophys., 13, 531-540
- Knopf, B., Zickfeld, K., Flechsig, M., Petoukhov, V. (2008): Sensitivity of the Indian monsoon to human activities. Advances in Atmospheric Sciences, 25/6, 932-945
- Van Oijen, M. et al. (2013): Bayesian calibration, comparison and averaging of six forest models, using data from Scots pine stands across Europe. Forest Ecology and Management, 289, 255-268
- Reyer, C., Flechsig, M., Lasch, P., van Oijen, M.: Integrating parameter uncertainty of a process-based model in assessments of climate change effects on forest productivity. Annals of Forest Science, in prep.

# Thank you for your Attention

PIK's Main Building (Michelson House)

http://www.pik-potsdam.de/software/simenv