Techniques for Quality Assurance of Models in a Multi-Run Simulation Environment

M. Flechsig[1] , U. Böhm[1] , T. Nocke[2] , C. Rachimow[1]

[1] PIK - Potsdam Institute for Climate Impact Research
[2] University of Rostock, Institute of Computer Graphics

TOPIK IV
Project ModSimEnv
Sub-Project SimEnv

General SimEnv Approach

SimEnv is a sampling-based simulation environment that enables model developers / users to deal with quality assurance matters and scenario analyses for any model M. It runs under Unix and Linux.

M: $y = F(X_k)$

$X_k = (x_1,...,x_k)$ input vector of factors (parameters, initial / boundary values)
y multi-dimensional (large scale) model output

SimEnv aims to support all stages of a model's life cycle (Fig. 1).

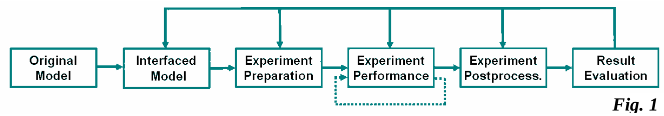
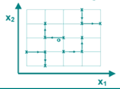
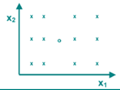
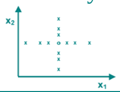
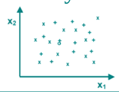
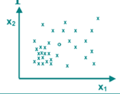


Fig. 1

Experiment Types

are the core of SimEnv. They represent different generic sampling strategies of the factor space $\{X_k\}$ formed from X_k and result in the performance of multi-run simulation experiments.
Generic experiment types have to be equipped with factors, a sample in the factor space, and a description of model output variables.

Global sensitivity analysis 	Qualitative ranking of a large number of factors with respect to their sensitivity on model output at random trajectories in the factor space $\{X_k\}$ For determination of most important factors to focus on afterwards
Behavioural analysis 	Deterministic inspection with a flexible screening strategy in the factor space $\{X_k\}$ For - one-factor-at-a-time experiments - (fractional) factorial experiments - response surface methodology
Local sensitivity analysis 	Deterministic sampling in a local neighbourhood of the default factor values of **M** For local first order sensitivity measures by investigating finite difference approximations of derivatives
Monte Carlo analysis 	Probabilistic random or Latin hypercube sampling of factors according to pre-defined distributions and determination of statistical measures For - error analysis - model validation
Uncertainty analysis 	Orthogonal variance decomposition of model output to first order and total effects by a Monte Carlo re-sampling experiment {+} (in prep.) For - uncertainty analysis - model validation
Optimization 	Stochastic sampling to find the global minimum of a cost function on $\{X_k\}$ applying the simulated annealing strategy ASA For model validation, control design: minimize a distance measure between model and data

{x}: sample set o: default factor value of **M** in $\{X_2\}$

Model Interface

is based on minimal source code modifications for C/C++, Fortran, Python, Matlab, Mathematica, and/or GAMS models, at UNIX shell level and for ASCII files by implementation of function calls

- to forward a sampled factor value x_i from SimEnv to **M**:
  one call of function **simenv_get** for each x_i
- to store model output y from **M** to SimEnv data structures:
  one call of function **simenv_put** for each y

SimEnv-related model output storage uses self-describing Network Common Data Form NetCDF or IEEE compliant binary formats.

Experiment Performance

- On local, remote, parallel or distributed hardware architectures (the latter two using Message Passing Interface MPI)
- Support of distributed models

Post-Processing and Visual Evaluation

Interactive post-processing allows

- to compute secondary output functions from the model's output y and from reference data by application of chains of elemental, selective, analytical, and statistical operators
- to navigate the factor space $\{X_k\}$ and derive from output functions uncertainty and sensitivity measures over the whole run ensemble by application of experiment type-specific operators

Currently, about 100 built-in operators are available. There is an interface to plug user-defined operators into the environment.

Analysis and evaluation of post-processed data derived from large amount of relevant model output benefit from coupled visualization techniques, using pre-defined OpenDX visualization modules.

Prospects

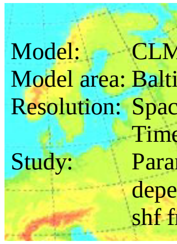
- Support of remotely coupled models by a SimEnv client - server architecture
- Single factor experiments as multi-factor experiment types
- Multi-file support for very large experiment output

References

ASA http://ingber.com/#ASA
CLM http://w3.gkss.de/CLM/clm_home.html
GAMS http://www.gams.com
MPI http://www.mpi-forum.org
NetCDF http://www.unidata.ucar.edu/packages/netcdf
OpenDX http://www.opendx.org

SimEnv on the Internet: http://www.pik-potsdam.de/software/simenv

Example



Model: CLM - regional meteorological model in climate mode
Model area: Baltic Sea and most of Northern and Central Europe
Resolution: Space: 0.5° lat x 0.5° lon x 20 vertical layers
Time: model time step: 90 sec, output: 6 hourly values
Study: Parametrization of the soil submodel: dependency of latent and sensible heat fluxes lhf and shf from soil in a $\{X_2\} = \{crs_{min} , T_{end}\}$ parameter space

Model output variable description file:

coordinate	lat	values	35 (0.5) 67	# defines coord. latitude with ½° resolution
coordinate	lon	values	-25 (0.5) 40	# defines coord. longitude
coordinate	time	values	1 (1) 28	# defines coord. time (6 hourly time steps)
variable	lhf	coords	lat , lon , time	# defines lhs as lhf(lat,lon,time)
variable	shf	coords	lat , lon , time	# defines shf as shf(lat,lon,time)

Experiment description file for a behavioural analysis in X_2:

factor	crsmin	sample	30. (5.) 120.	# specifies 19 sampled values for crs_{min}
factor	crsmin	default	60.	# default model value of crs_{min}
factor	crsmin	type	set	# do not modify sampled values by def. val
factor	Tend	sample	273.15 (5) 333.15	# specifies 13 sampled values for T_{end}
factor	Tend	default	313.15	
factor	Tend	type	set	
specific		comb	crsmin*Tend	# factorial screening: 1+19*13=248 runs

Post-processor operator chain:

Fig. 2:	behav(' ', avg(shf)) - run('default', avg(shf))	# area- and temporal averaged shf anomaly
Fig. 3:	behav('sel_s(Tend=313.15)', avg_l('time', shf)) - run('default', avg_l('time', shf))	# area-averaged shf anomaly for each time step, all crs_{min}, and the def. value of T_{end}

Fig. 2

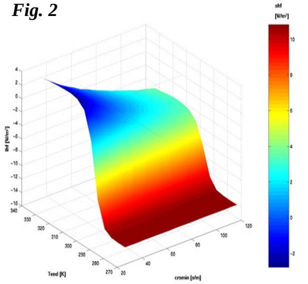
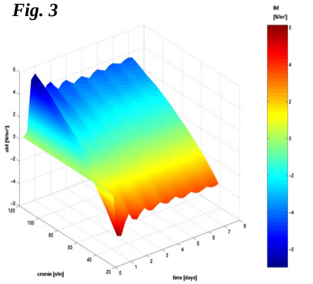


Fig. 3



Experiment: Monte Carlo analysis in X_2 for model time steps 2 - 28
crs_{min} , T_{end} ~ N(def_value,20.), Latin hypercube sampling, 150 runs:

Fig. 4: pdf of lhf anomaly per time step
bin range = [-5.02 , 2.03]

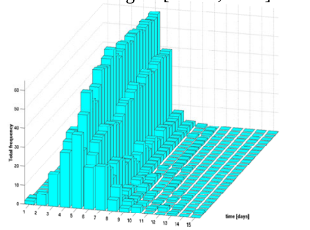


Fig. 5: pdf of shf anomaly per time step
bin range = [-1.51 , 3.87]