Hydroinformatik - SoSe 2024
HyBHW-S1-01-V10: Hydrologische Modellierung

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3. Hydro-System Modelle
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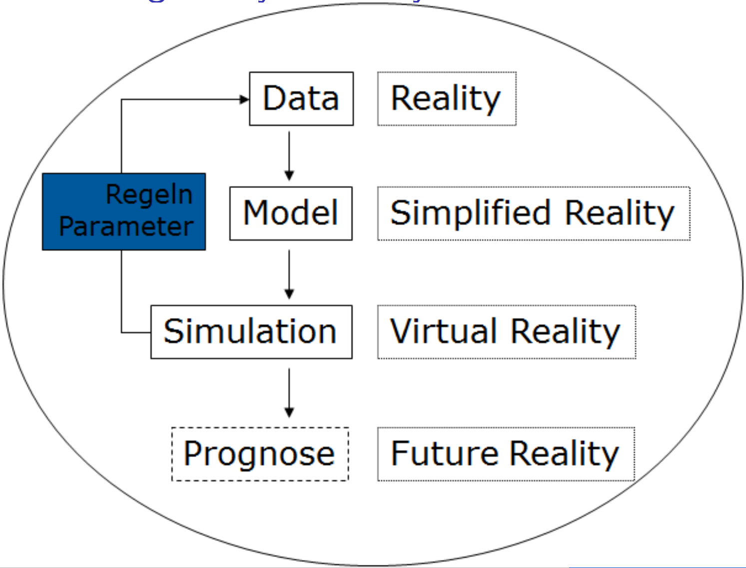
5. "Surrogate" Modelle
6. (professional) Work Flows ...

Modell-Begriff

Modell-Begriff: Systemanalyse



$\hookrightarrow$ Kalibrierung $\longrightarrow$
Validierung $\longrightarrow$
Verfizierung (A & B) $\hookleftarrow$

Modell-Begriff: Publikation: Görke et al. (2015)

[illegible]

ON THE TERM AND CONCEPTS OF NUMERICAL MODEL VALIDATION IN GEOSCIENTIFIC APPLICATIONS

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Key words: Coupled Problems, Model Development, Numerical Methods, Model Calibration, Inverse Problems

Abstract. Modeling and numerical simulation of the coupled physical and chemical processes observed in the subsurface are the only options for long-term analyses of complex geological systems. This contribution discusses some more general aspects of the advanced process modeling for geoscientific applications including reflections about the slightly different understanding of the terms *model* and *model validation* in different scientific communities, and about the term and methods of *model calibration* in the geoscientific context. Starting from the analysis of observations of a certain part of the perceived reality, the process of model development comprises the establishment of the physical model characterizing relevant processes in a problem-oriented manner, and subsequently the mathematical and numerical models. Considering the steps of idealization and approximation in the course of model development, Oreskes et al. [1] state that process and numerical models can neither be verified nor validated in general. Rather the adequacy of models with specific assumptions and parameterizations made during model set-up can be confirmed. If the adequacy of process models with observations can be confirmed using lab as well as field tests and process monitoring, the adequacy of numerical models can be confirmed using numerical benchmarking and code comparison. Model parameters are intrinsic elements of process and numerical models, in particular constitutive parameters. As they are often not directly measurable, they have to be established by solving inverse problems based on an optimal numerical adaptation of observation results. In addition, numerical uncertainty analyses should be an obligatory part of numerical studies for critical real world applications.

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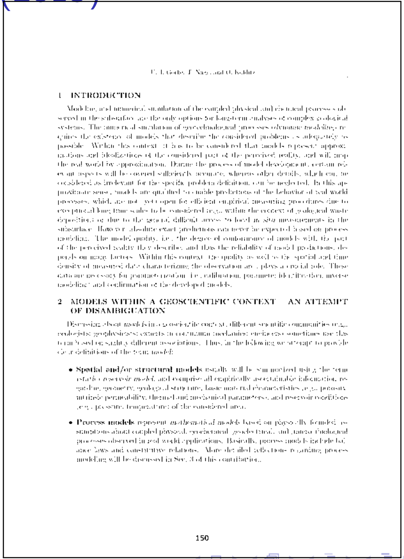

U.-J. Görke, T. Nagel and O. Kolditz

1 INTRODUCTION

Modeling and numerical simulation of the coupled physical and chemical processes observed in the subsurface are the only options for long-term analyses of complex geological systems. The numerical simulation of geotechnological processes (*dynamic modeling*) requires the existence of models that describe the considered problems as adequately as possible. Within this context, it has to be considered that models represent approximations and idealizations of the considered part of the perceived reality, and will map the real world by approximation. During the process of model development, certain relevant aspects will be covered sufficiently accurate, whereas other details, which can be considered as irrelevant for the specific problem definition, can be neglected. In this approximate sense, models are qualified to enable predictions of the behavior of real world processes, which are not (yet) open for efficient empirical measuring procedures due to exceptional long time scales to be considered (e.g., within the context of geological waste deposition) or due to the general difficult access to local *in situ* measurements in the subsurface. However, absolute exact predictions can never be expected based on process modeling. The model quality, i.e., the degree of conformance of models with the part of the perceived reality they describe, and thus the reliability of model predictions, depends on many factors. Within this context, the quality as well as the spatial and time density of measured data characterizing the observation area plays a crucial role. These data are necessary for parameterization (i.e., calibration, parameter identification, inverse modeling) and confirmation of the developed models.

2 MODELS WITHIN A GEOSCIENTIFIC CONTEXT – AN ATTEMPT OF DISAMBIGUATION

Discussing about *models* in a geoscientific context, different scientific communities (e.g., geologists, geophysicists, experts in continuum mechanics, engineers) sometimes use this term based on slightly different associations. Thus, in the following we attempt to provide clear definitions of the term *model*:

- **Spatial and/or structural models** usually will be summarized using the term (*static*) *reservoir model*, and comprise all empirically ascertainable information regarding geometry, geological structure, basic material characteristics (e.g., porosity, intrinsic permeability, thermal and mechanical parameters), and reservoir conditions (e.g., pressure, temperature) of the considered area.
- **Process models** represent *mathematical models* based on physically founded assumptions about coupled physical, geochemical, geotechnical, and partly biological processes observed in real world applications. Basically, process models include balance laws and constitutive relations. More detailed reflections regarding process modeling will be discussed in Sec. 3 of this contribution.

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Modell-Begriff

Definition

"Modeling and numerical simulation of the coupled physical and chemical processes observed in the subsurface are the only options for long-term analyses of complex geological systems. The numerical simulation of geotechnological processes (dynamic modeling) requires the existence of models that describe the considered problems as adequately as possible. Within this context, it has to be considered that models represent approximations and idealizations of the considered part of the perceived reality, and will map the real world by approximation. During the process of model development, certain relevant aspects will be covered sufficiently accurate, whereas other details, which can be considered as irrelevant for the specific problem definition, can be neglected. In this approximate sense,

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Modell-Begriff

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Modell-Abstraktion

Geo-Systeme $\Rightarrow$ Hydro-Systeme

Modell-Begriff

Klassifikation

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- **Process models** represent mathematical models based on physically founded assumptions about coupled physical, geochemical, geoelectrical, and (micro-)biological processes observed in real-world applications. Basically, process models include balance laws and constitutive relations. More detailed reflections regarding process modeling will be discussed in Sec. 3 of this contribution.

Modell-Begriff

Klassifikation

- **Numerical models:** The field equations based on balance laws including relevant constitutive relations can be solved analytically just in exceptional cases. Corresponding specific problems frequently will be defined in terms of benchmarks for model and software confirmation. Usually, the solution of field equations describing a real-world problem requires the use of numerical methods. For that, the local formulation of balance laws in terms of differential equations has to be transformed into a global integral formulation. In general, the resulting system of equations is a nonlinear one and contains time derivatives of the primary variables to be calculated. As numerical methods do not provide spatially and temporally continuous solutions, but rather solutions in discrete points of the given solution space, the system of field equations including constitutive relations has to be discretized in space and time within the context of incremental-iterative approximation procedures. In addition, nonlinear systems have to be linearized. The resulting so-called initial-boundary value problem can be solved numerically in discrete locations at discrete points of time. As spatial discretization approaches, the methods of finite differences (FDM), finite volumes (FVM), and finite elements (FEM) are widely excepted means of choice.

Modell-Begriff

Numerische Modelle

Within this context, the term numerical model characterizes either

- numerical methods and algorithms necessary for **computer-based simulations** of the process model, or
- the **entire data set** necessary for the numerical simulation of a specific problem (parameterized and spatially discretized structural model; boundary and initial conditions; parameters controlling the simulation procedure).

Modell-Begriff

Process Modeling

The process modeling of physical, geochemical, and (micro-)biological processes in the subsurface is based on mathematical theories enabling the description of spatially and temporally evolving processes of the perceived reality in terms of differential equations or systems of differential equations. Developing the relevant mathematical apparatus, we make use of physically, chemically, and biologically founded assumptions.

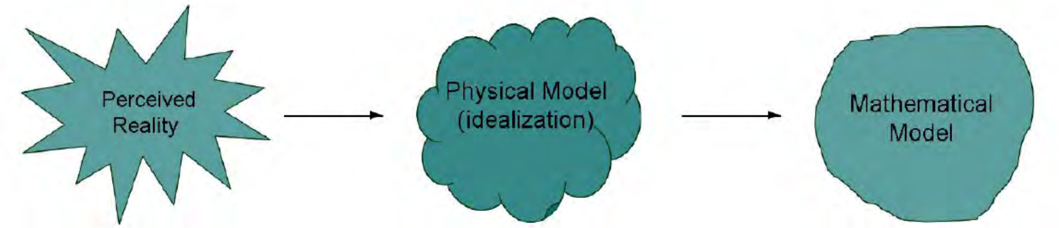


Figure: Model generation

Modell-Begriff

Model Confirmation

The procedure of the development of process models illustrated in Sec. 3 shows that models are always idealizations and approximations of a considered part of the perceived reality reflecting specific assumptions and parameterizations made for the model set-up. In order to assure the usability of a process model and the corresponding numerical model, it has to be shown that it adequately reflects real-world processes. In the literature, this process is called **model validation** or even **model verification** – but are these terms justified in their absolute, literal meaning?

Modell-Begriff

Model Confirmation

- **Model verification** ". . . means an assertion or establishment of truth." and "To say that a model is verified is to say that its truth has been demonstrated, which implies its reliability as a basis for decision-making."
- **Model validation** ". . . does not necessarily denote an establishment of truth. . . Rather, it denotes the establishment of legitimacy. . . " and ". . . a model that does not contain known or detectable flaws and is internally consistent can be said to be valid."

Source: Oreskes, N., Shrader-Frechette, K. and Belitz, K. Verification, Validation, and Confirmation of Numerical Models in the Earth Sciences. Science (1994) 263:641–646.

Modell-Begriff

Model verification ?

- ". . . models. . . are never closed systems" (but truth can be demonstrated only for closed systems),
- models ". . . require input parameters that are incompletely known",
- data sets for the parameterization (i.e., calibration) of process models are always incomplete (e.g., due to the availability of only a few locally determined parameters from core tests considering a model of a whole geological reservoir), and
- often used phenomenological constitutive theories are characterized by loss of information on real physical scale (e.g., use of macroscale models not being based on real microscale behavior),

Modell-Begriff

Model validation ?

Legitimacy of a model:

- model results depend on assumptions required for model development and on parameterization, and
- models valid for one mapping of the reality may not be valid for another one (e.g., material behavior dependent on temperature).

Modell-Begriff

Model calibration !

If the terms model verification and model validation are unfavorable in their literal meaning, how else the usability of process models can be assured? For this purpose, Oreskes et al. introduce the term model calibration stating: ". . . science requires that empirical observations be framed as deductive consequences of a general theory. . . If these observations can be shown to be true, the theory. . . is confirmed. . . ", and ". . . confirming observations do not demonstrate the veracity of a model. . . , they only support its probability." Thus, rather the adequacy of models with specific assumptions and parameterizations made during model set-up can be confirmed, not their (general) truth. Within this context, model parameterization is performed using well-established approaches of model calibration. If the adequacy of process models with observations can be confirmed using lab as well as field tests and process monitoring, the adequacy of numerical models can be confirmed using numerical benchmarking (e.g., providing analytical solutions) and code comparison for more complex systems.

Modell-Begriff

Model calibration

Model parameters, in particular constitutive parameters, are constituent, intrinsic elements of process and numerical models. Parameterized models are used for simulations in order to analyze and/or predict the evolution of various processes in real-world applications, thus, solving a direct problem (cf. Fig. 4).

Figure: Direct modeling: simulation of real-world problems using parameterized process and numerical models

Modell-Begriff

Model optimization

As model parameters are often not directly measurable, their identification is based on the analysis of their effects onto measurable field variables. This process of model calibration (i.e., model parameterization) requires the solution of an inverse problem based on an optimal numerical adaptation of observation results (cf. Fig. 5).

Figure: Inverse modeling: optimal numerical adaptation of observations from lab and field experiments, and from field exploration

Modell-Begriff

Objective function

A model function will be defined, which characterizes an arbitrary field variable y depending on a vector of variables $\boldsymbol{x}$ as well as on a set (vector) of model parameters $\boldsymbol{c}$

$$y = y(\boldsymbol{x}, \boldsymbol{c}) \tag{1}$$

Norms:

$$\frac{1}{2} \sum_{i=1}^{n} = [\hat{y}_i^2 - y^2(\boldsymbol{x}, \boldsymbol{c})] \rightarrow \min \tag{2}$$

Residuals:

$$\boldsymbol{r}(\boldsymbol{c}) = \{r_i(\boldsymbol{c})\} \quad \text{with} \quad r_i(\boldsymbol{c}) = \hat{y}_i - y(\boldsymbol{x}_i, \boldsymbol{c}) \tag{3}$$

Modell-Begriff

Objective function

Objective function

$$\Phi(\boldsymbol{c}) = \frac{1}{2}\boldsymbol{r}^T(\boldsymbol{c})r(\boldsymbol{c}) = \frac{1}{2}\sum_{i=1}^{n} = \hat{r}_i^2(\boldsymbol{c}) \rightarrow \min \qquad (4)$$

Optimality criterion

$$\nabla\Phi(\boldsymbol{c}^*) = 0 \qquad (5)$$

Normal equation

$$\boldsymbol{J}^T\boldsymbol{J}\boldsymbol{c}^* = \boldsymbol{J}^T\boldsymbol{r} \qquad (6)$$

Jacobian matrix

$$\boldsymbol{J} \qquad (7)$$

Modell-Begriff

Conclusions

Following aspects are important to reliable process simulations:

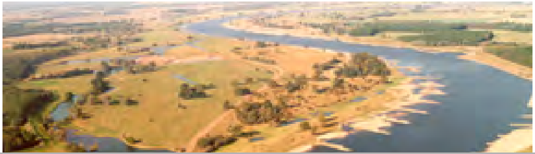
- Definition of the **processes and subprocesses** that are relevant for the specific problem to be solved in order to establish a system of field equations, which is complex enough to cover the relevant system behavior but simple enough to ensure an efficient and stable solution process.
- Formulation of problem-dependent specific expressions of the balance laws and the constitutive relations according to the latest state of research.
- Model confirmation using standardized **benchmarks and code comparison**.
- Extensive provision of **data** from lab and field tests for an improved process understanding and for the model calibration.
- If measured data are not available for all local points of the spatially discretized observation area (this is the usual case for geoscientific real-world applications), a stochastically based parameter space has to be determined based on a statistically sufficient number of different numerical realizations.
- An **uncertainty analysis** is advised based on this parameter space, and results of the process simulation will be provided with certain likelihood.

Hydro-Systeme

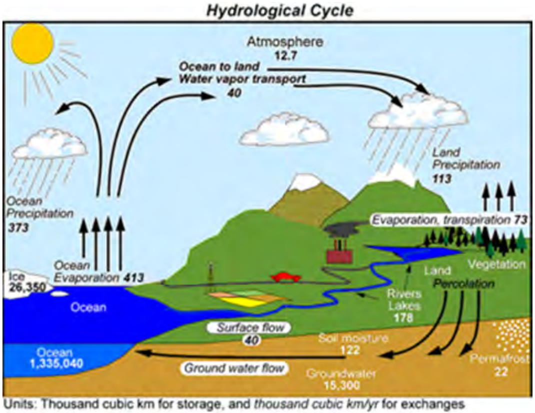
Hydrosysteme

Totes Meer (Dead Sea) - Arid

Elbe - Humid



Wasserkreislauf



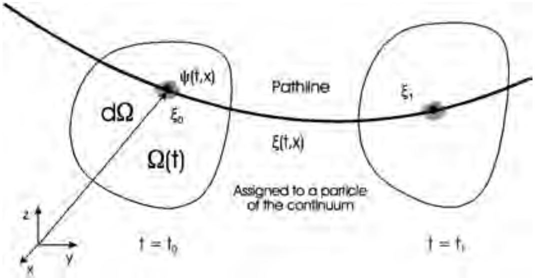
Hydro-System Modelle

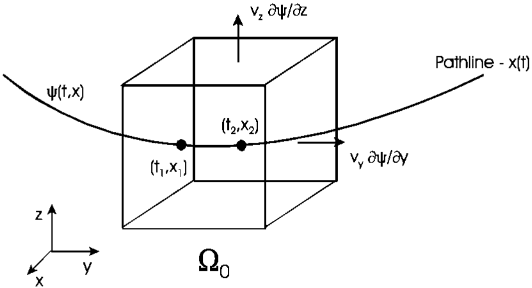
- Prozess-basierte Modelle
- Surrogate (daten-basierte) Modelle

Prozessbasierte Modelle

Prozessbasierte Modelle

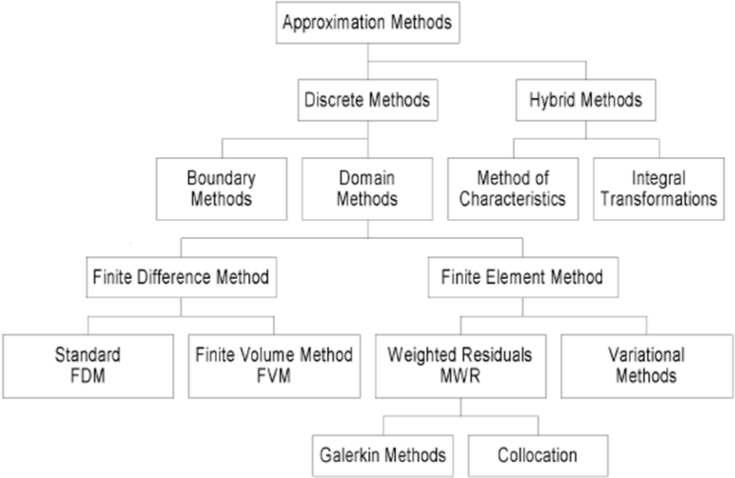
>> nächstes Semester - Hydroinformatik II





Prozessbasierte Modelle

>> nächstes Semester - Hydroinformatik II



Prozessbasierte Modelle

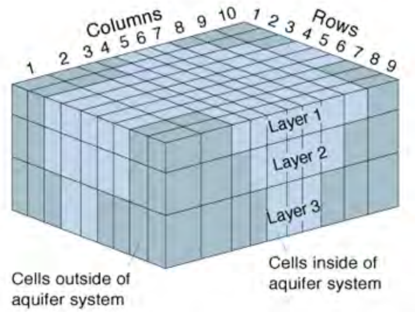
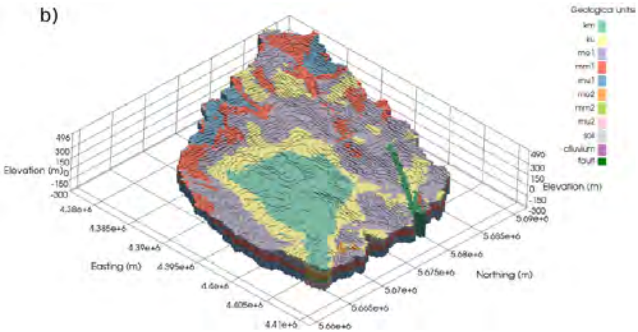
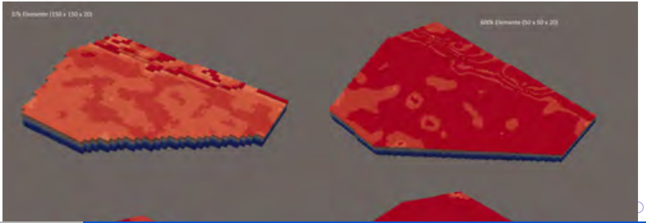


Figure 2. Example of model grid for simulating three-dimensional ground-water flow.

MODFLOW (↑)

OpenGeoSys-Modelle



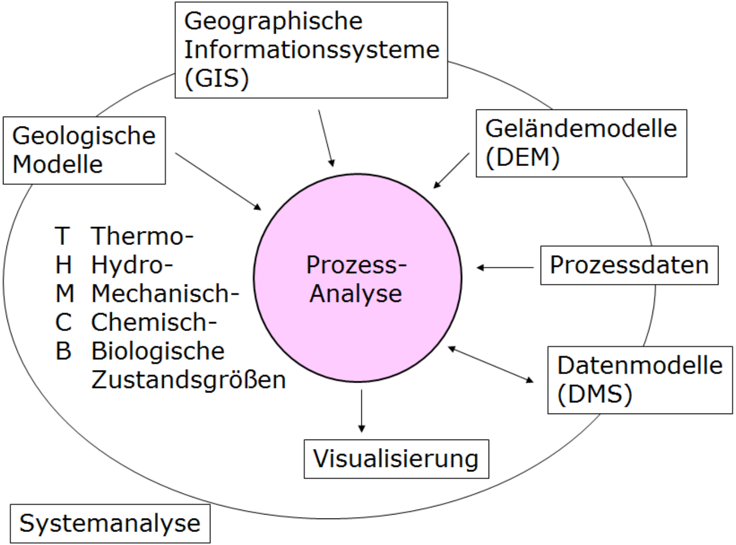


"Surrogate" Modelle

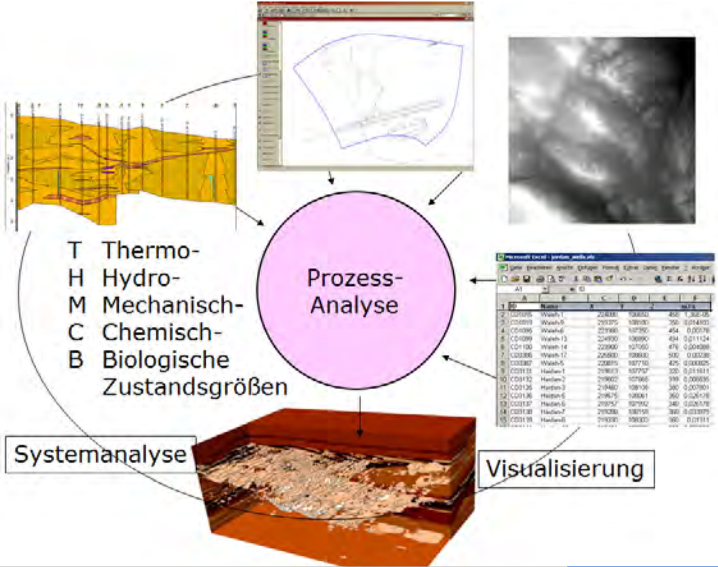
- Stochastische Modelle
- Netzwerke (Neuronale, Bayes'sche Netzwerke, ...)
- Machine Learning (KI)
- ...

Work Flows ...

Work Flows


Geographische Informationssysteme (GIS)
Geologische Modelle
Geländemodelle (DEM)
T Thermo-
H Hydro-
M Mechanisch-
C Chemisch-
B Biologische
Zustandsgrößen
Prozess-Analyse
Prozessdaten
Datenmodelle (DMS)
Visualisierung
Systemanalyse

Work Flows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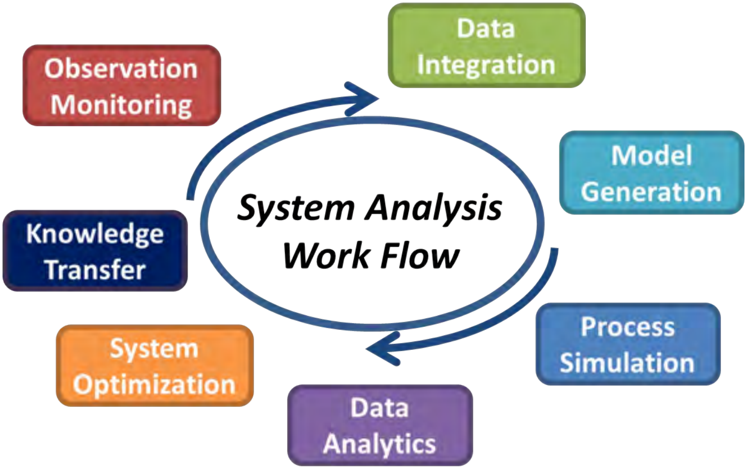
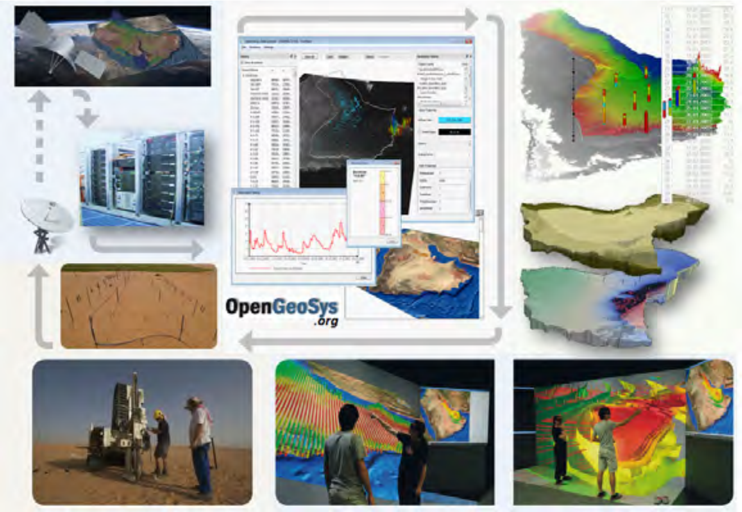
Prozess-
Analyse
Systemanalyse
Visualisierung

Work Flows: Generic Concept



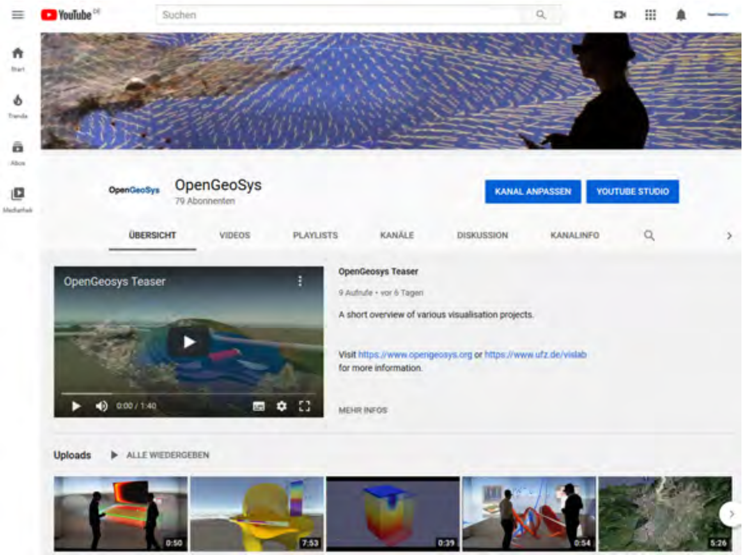
Object Orientation

Work Flows: Hydrosystems

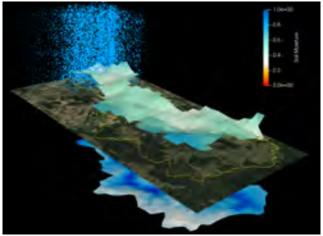


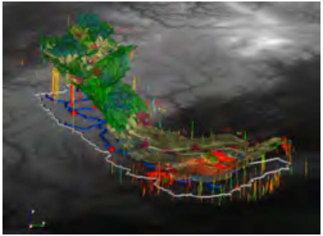
Quelle: Kalbacher et al. (2012)

Visualisierung: Lars Bilke und Karsten Rink



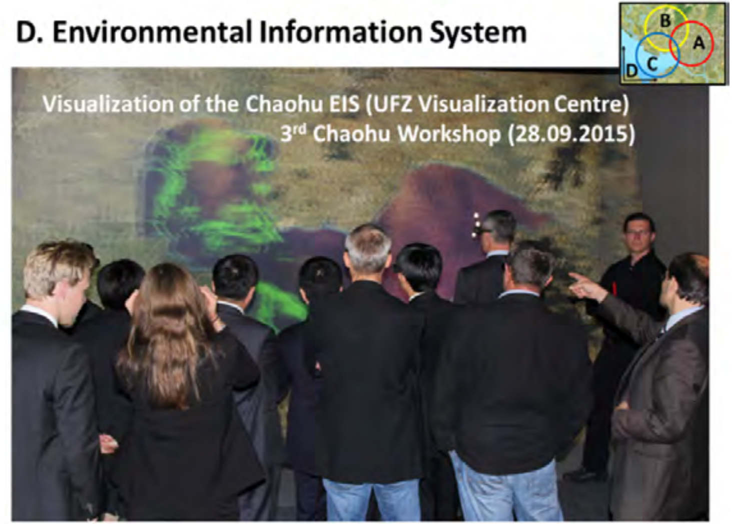
https://www.youtube.com/user/OpenGeoSys

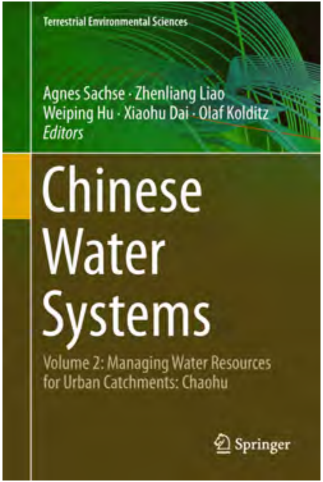




CAWR Project: "Urban Catchments"

Visualisierung: Karsten Rink





DFG#NSFC Project: "Poyang Lake"

Visualisierung: Karsten Rink