Hydroinformatik I - WiSe 2020/2021 HyBHW-S1-01-V9: Hydrologische Modellierung

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Dresden, 08.01.2021

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08.01.2021

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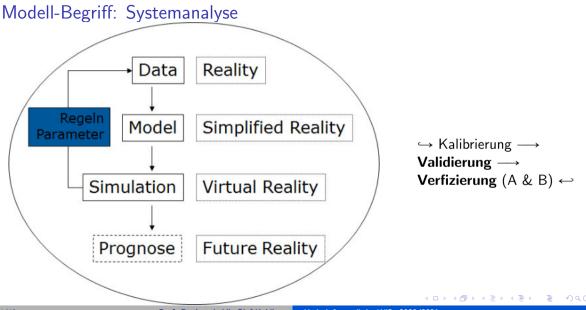
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Modell-Begriff: Publikation: Görke et al. (2015)

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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,

Görke, U.-J., Nagel, T., Kolditz, O., (2015): On the term and concepts of numerical model validation in geoscientific applications In: Schrefler, B., Oñate, E., Papadrakakis, M., (eds.) Proceedings of the 6th International Conference on Computational Methods for Coupled Problems in Science and Engineering - COUPLED PROBLEMS 2015, CIMNE, 18 - 20 May 2015, San Servolo, Venice, Italy

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Modell-Begriff

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... models are gualified 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."

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Modell-Abstraktion

$\mathsf{Geo}\text{-}\mathsf{Systeme} \Rightarrow \mathsf{Hydro}\text{-}\mathsf{Systeme}$

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Modell-Begriff

Klassifikation

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, 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.

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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

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Modell-Begriff Numerische Modelle

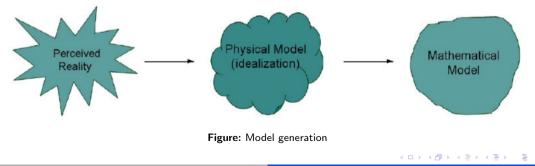
Within this context, the term numerical model characterizes either

- 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.



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?

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.

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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),

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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).

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Model calibration 1

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.

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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).

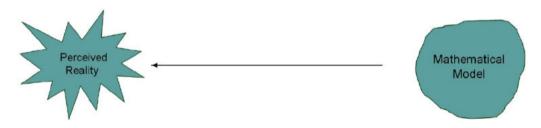


Figure: Direct modeling: simulation of real-world problems using parameterized process and numerical models

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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

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Objective function

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

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

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Norms:

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

Residuals:

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

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Modell-Begriff

Objective function

Objective function

$$\Phi(\boldsymbol{c}) = \frac{1}{2}\boldsymbol{r}^{\mathsf{T}}(\boldsymbol{c})\boldsymbol{r}(\boldsymbol{c}) = \frac{1}{2}\sum_{i=1}^{n} = \hat{r}_{i}^{2}(\boldsymbol{c}) \to \min$$
(4)

Optimality criterion

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

Normal equation

$$\boldsymbol{J}^{\mathsf{T}}\boldsymbol{J}\boldsymbol{c}^* = \boldsymbol{J}^{\mathsf{T}}\boldsymbol{r} \tag{6}$$

(7)

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Jacobian matrix

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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. ・ロト ・雪 ト ・ ヨ ト ・ ヨ ト

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Hydro-Systeme

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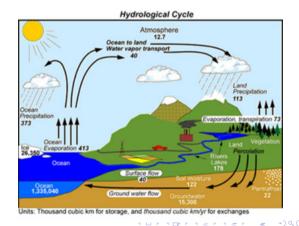


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Prof. Dr.-Ing. habil. Olaf Kolditz

Wasserkreislauf



Hydro-System Modelle

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

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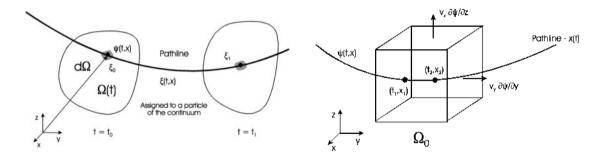
Prozessbasierte Modelle

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Prozessbasierte Modelle

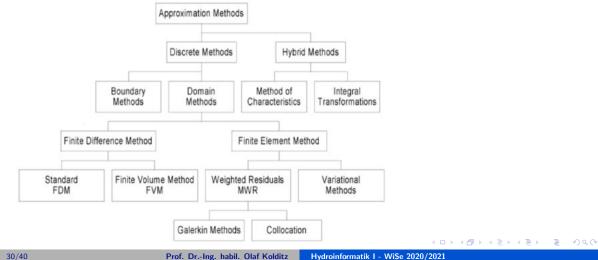
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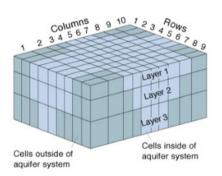
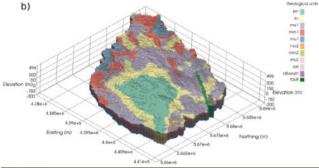
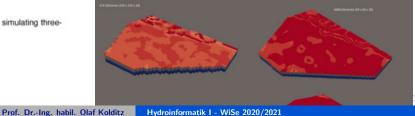


Figure 2. Example of model grid for simulating threedimensional ground-water flow.

MODFLOW (↑)

OpenGeoSys-Modelle





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

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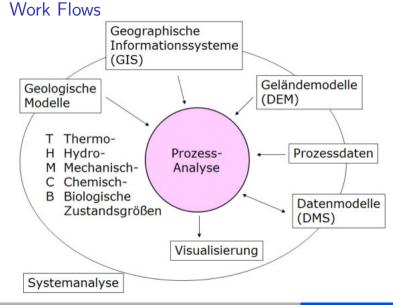
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Work Flows ...

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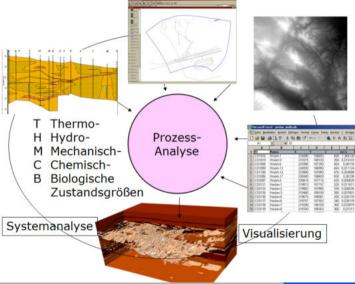




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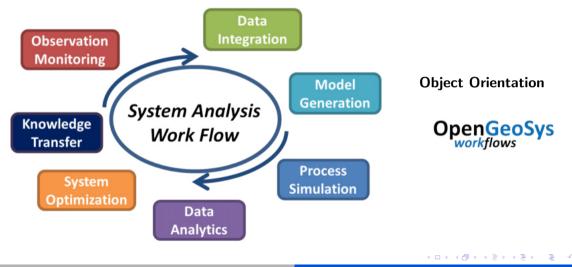


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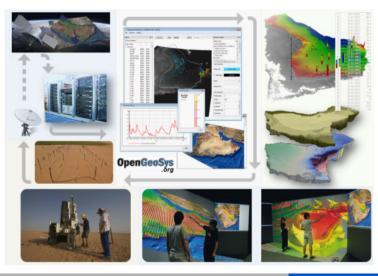
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Work Flows: Generic Concept



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Work Flows: Hydrosystems



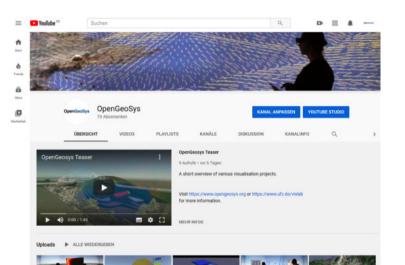
Quelle: Kalbacher et al. (2012)

Visualisierung: Lars Bilke und Karsten Rink

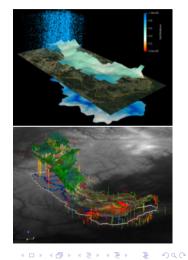
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https://www.youtube. com/user/OpenGeoSys



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CAWR Project: "Urban Catchments"

D. Environmental Information System



Visualization of the Chaohu EIS (UFZ Visualization Centre) 3rd Chaohu Workshop (28.09.2015)

Visualisierung: Karsten Rink

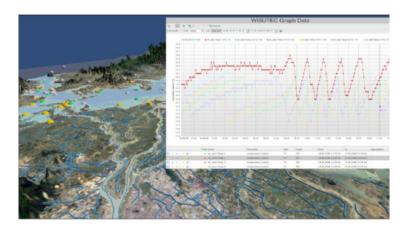


Chinese Water Systems

Volume 2: Managing Water Resources for Urban Catchments: Chaohu

DFG#NSFC Project: "Poyang Lake"

Visualisierung: Karsten Rink





Chinese Water Systems

Volume 3: Poyang Lake Basir

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