Friedrich-Alexander-Universität Erlangen-Nürnberg

RecHierarchicalIdent

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Recursive and Hierarchical Identification on Reactive Transport and Fluid Flow Models

1. Project

Recent challenges like bioremediation, longterm underground storage of reactive waste or underground carbondioxids sequestration require more and more complex multicomponent reactive transport models. Although being demanding concerning their numerical approximation, the decisive bottleneck in using such a model seems to lie in the **availability of the increasing range of the corresponding reaction parameters**.

The subject of this project is the investigation of possible identification problems for such flow and reactive transport applications in porous media, including, e.g., the **van Genuchten parametrization** for hydraulic properties and the **Monod Model** for biodegradation. Depending on the considered situation (laboratory or field cases, saturated and/or vadose zone, various phases and multiple interacting species) and the design of experimental models of varying complexity may be necessary. A typical example includes contaminant transport in the vadose zone modelled by the **Richards equation coupled to several advection-diffusion-reaction-equations**.

The aim of this project is to examine **various identification strategies for the inverse problem** improving the standard least squares approaches. Hierarchical choices of parameter sets, multi experimental design, **formfree procedures embedded into a multi-level algorithm**, regularized parameter functions in case of numerical difficulties and **sensitivity considerations in the residuum** are investigated. The concepts will be illustrated by outflow and breakthrough experiments with soil columns. Thereby, it is wellknown that the sensitivity and the correlation of parameters prevent a reliable reconstruction from naive history matching.

3. Identification

For the identification of unknown material properties, respected in the model by unknown coefficient functions $p\in P$, a finite number $\kappa\in\mathbb{N}$ of selected experiments e_k can be accomplished. Since the continuous solution of the direct problem will not be measurable at a practical realization, only a couple of characteristic model parameters w_{ki} and error afflicted measurements $g_{\varepsilon,ki}$ are available. An obvious approach for the identification is the minimization of the (weighted) ordinary least squares (OLS) functional

$$\mathcal{J}_\varepsilon(p)=\sum_{k=1}^{\kappa}\sum_{i=1}^{n_k}\Lambda_i(g_{\varepsilon,ki})\Big\|w_{ki}(p)-g_{\varepsilon,ki}\Big\|_2^2 .$$

For solving the optimization problem, derivative-free as well as linearizing techniques, such as the SQP-method, can be applied. But, because of the complexity and the high nonlinearity, just a trapping to a local minimum can be expected in case of a fixed experimental setup. Furthermore, because of existing data and observation errors, it has to be attended that a decreasing functional does not enforcedly lead to a decreasing identification error. To counteract this behavior, a systematic use of the singular values

$$(\lambda_{ki})_j(p_0):=\sqrt{\sum_{l=1}^{r}\Big(\big(S_{ki}^{+}\big)_{lj}(p_0)\Big)^2}$$

of the sensitivity matrices $S_{ki}\in\mathbb{R}^{m_{ki},r}$ in the definition of the discrete error functional

$$\mathcal{J}_{h,\varepsilon}(p;p_0)=\sum_{k=1}^{\kappa}\sum_{i=1}^{n_k}\Lambda_{ki}(g_{h_\varepsilon,ki})\sum_{j=1}^{m_{ki}}\lambda_{ki,j}(p_0)\big(w_{ki,j}(p)-g_{\varepsilon,ki,j}\big)^2$$

is used. Hence, an adaptive approach is designed in which after each termination in a local minimum the sensitivity based weights, and with it the error functional, are modified. There is no mathematical proof for convergence but almost all numerical examples (the number of unknowns must not be to large) show in comparison with the standard OLS a significantly decreasing identification error.

Unfortunately, inverse problems are often ill-posed (e.g. with regard to the Richards equation with van Genuchten parametrization or the entire Monod reaction rate) such that an ordinary or even recursive OLS approach leads only conditionally to satisfying results. For this kind of problems an alternative formfree ansatz will be applied in which a set of spline approximations $f_{\vec r}^{j}$ is used to specify an unknown nonlinearity $f:\mathbb{R}^d\to\mathbb{R}^d$. Since, in case of a high number of degrees of freedom, the minimization of the error functional is highly sensitive to the initial values and the convergence is accordingly slow, the formfree procedure is embedded into a multi-level algorithm[1] where

$$f_{\vec r}^{j}(\vec x)=\sum_{\vec\nu\in N_d(\vec r)}p_{\vec r,\vec\nu}^{j}\Phi_{\vec r,\vec\nu}^{j}(\vec x)\,,\quad \Phi_{\vec r,\vec\nu}^{j}\ \text{basis of}\ P_{\vec r}^{j}\,,\quad p_{\vec r,\vec\nu}^{j}\in\mathbb{R}\,,\quad j=1,\dots,d,$$

holds for stepwise increasing $\vec r\in\mathbb{N}^d$,

$$N_d(\vec r)=\Big\{\vec\nu\in\mathbb{N}^d\,\big|\,\nu_i\le r_i\,\forall\, i=1,\dots,d\Big\},$$

and vector spaces $P_{\vec r}^{j}$ of polynomials of maximal degree of freedom of $r=\Pi_{i=1}^{d}$,

$$P_{\vec r}^{j}\subset P_{\vec r'}^{j},\quad \vec r\le\vec r'\ \text{(componentwise)}\quad\text{and}\quad \overline{\bigcup_{\vec r\in\mathbb{N}^d}P_{\vec r}^{j}}=P^{j}.$$

In case of a multi-dimensional parametrization (e.g. $d=3$ for the entire Monod reaction rate) sparse grids are used for a further simplification by a significant decreasing of the degree of freedom.

1) for a 1D notation see e.g. B. Igler. *Identification of Nonlinear Coefficient Functions in Reactive Transport through Porous Media*, Dissertation, University of Erlangen, 1998.

2. Model Equation

The mathematical model consists of a description of the (un-)saturated water flow and, in case of reactive components, of a transport formulation. The flow given by the Richards equation reads

$$\partial_t\theta+\nabla\cdot q=0\,,\quad q=-K\nabla(\psi+h)\,,$$

with parametrization of the water retention curve $\theta(\psi)$ and the unsaturated hydraulic conductivity $K(\psi)$. The fixed parameterization

$$\theta(\psi)=\theta_{\text{res}}+(\theta_{\text{sat}}-\theta_{\text{res}})\Phi(\psi)\,,$$

$$K(\Phi)=K_{\text{sat}}\sqrt{\Phi(\psi)}\Big(1-\big(1-\Phi(\psi)^{\frac{1}{m}}\big)^m\Big)^2,$$

$$\Phi(\psi)=\frac{1}{\big(1+(-\alpha\psi)^n\big)^m}\,,\quad m=1-\frac{1}{n}\,,$$

given by the van Genuchten ansatz is besides other approaches widespread, but using formfree nonlinearities instead of fixed parametrization is also possible and favorable. The general transport equation for each reactive component c_i reads

$$\partial_t\big(\theta(x,t)c_i(c,t)\big)-\nabla\cdot\big(D_i(x,t)\nabla c_i(x,t)-\varphi_i(x,t)c_i(x,t)\big)=R_i\,.$$

In case of the three component Monod model, the reaction term for the mobile donator c_D and acceptor c_A as well as the immobile biomass c_B reads

$$R_{A,B,D}=\mu_{\max}\left(\frac{c_D}{K_{M_D}+c_D+\frac{c_D^2}{K_{ID}}}\right)\left(\frac{c_A}{K_{M_A}+c_A+\frac{c_A^2}{K_{IA}}}\right)c_B$$

with additional yieldfactors $\alpha_{A/D}$ and Y for R_A and R_B respectively and an optional penalty term $\big(1-\frac{c_B}{c_{B\max}}\big)$ for the biomass.

4. Numerical Results

Firstly, a virtual (Monod-)experiment with unknown parameters K_{M_D}, K_{I_D}, K_{M_A}, $\mu_{\max}$, Y and $\alpha_{A/D}$ is identified by the standard OLS ansatz as well as by the adaptive approach with weighting factors based on the pseudoinverse sensitivity matrices. The necessary measurements are defined by virtually generated breakthrough curves of the donator and acceptor both exact and disturbed (by 5% random noise). Figure 1 provides for the non-error afflicted computation the obtained Euclidean-norms for an increasing number of recursive identification starts. Figure 2 presents for the disturbed example the improvement of the achieved parameters. The decisive performance advantage of the new method is in both cases highly visible.

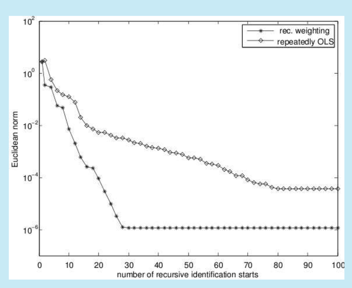

Figure 1: Euclidean-norms

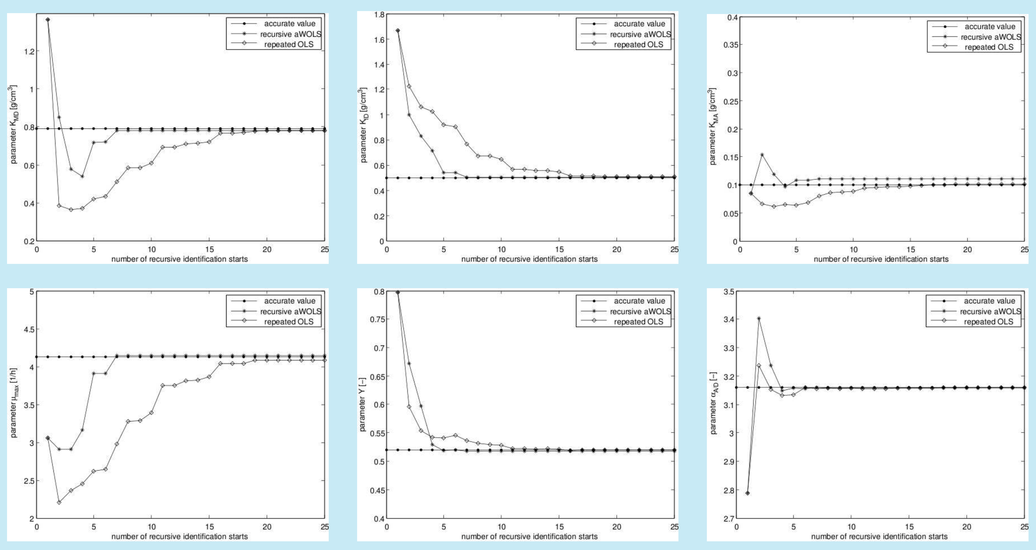

Figure 2: Recursive Identification of six Monod-Parameters

A second promising application was dealing with the identification of a global parametrization from a (real) soil column outflow experiment which was accomplished by the group of Tom Schanz at the Bauhaus-University of Weimar. Because of numerical difficulties induced by the van Genuchten parametrization, a regularization of the soil hydraulic properties was used, leading to a robust reconstruction of the pressure curves. Contrary to the standard approach, the new adaptive ansatz also provides quite similar results for different sets of available measurement data.

	IC	OLS	rec 5	rec 10	rec 15	rec 20	rec 30	rec $\geq$ 37
α	0.02	0.0391	0.0385	0.0384	0.0383	0.0382	0.0381	0.0371
n	3.0	4.5728	4.4775	4.2653	4.1042	3.9149	3.7469	3.6466
θ_{res}	0.05	0.0973	0.1057	0.1183	0.1279	0.1391	0.1490	0.2070
max		$4.93\cdot10^0$	$4.92\cdot10^0$	$4.95\cdot10^0$	$4.97\cdot10^0$	$4.99\cdot10^0$	$5.02\cdot10^0$	$5.01\cdot10^0$
Eucl		$2.93\cdot10^1$	$2.93\cdot10^1$	$2.94\cdot10^1$	$2.95\cdot10^1$	$2.96\cdot10^1$	$2.97\cdot10^1$	$2.97\cdot10^1$
func		$8.59\cdot10^2$	$8.59\cdot10^2$	$8.65\cdot10^2$	$8.70\cdot10^2$	$8.77\cdot10^2$	$8.84\cdot10^2$	$8.84\cdot10^2$

Table 1: Identification with only pressure measurements

	IC	OLS	rec 2	rec 4	rec 6	rec $\geq$ 8
α	0.02	0.039625	0.039122	0.039185	0.039144	0.039137
n	3.0	3.690272	3.744265	3.713031	3.687270	3.667625
θ_{res}	0.05	0.100471	0.099292	0.101756	0.103788	0.105338
max		$5.08\cdot10^0$	$5.05\cdot10^0$	$5.06\cdot10^0$	$5.06\cdot10^0$	$5.07\cdot10^0$
eucl		$3.01\cdot10^1$	$3.00\cdot10^1$	$3.00\cdot10^1$	$3.01\cdot10^1$	$3.01\cdot10^1$
func		$9.07\cdot10^2$	$9.01\cdot10^2$	$9.03\cdot10^2$	$9.04\cdot10^2$	$9.05\cdot10^2$

Table 2: Using with pressure and water content data

Finally, a formfree identification result[2] for an approximation with quadratic B-Splines and 10 degrees of freedom for every function is shown in figure 3. The necessary measurements were provided by a direct problem based on the van Genuchten parametrization. To simulate a realistic scenario the data was disturbed by a 5% Gaussian noise. In spite of the error afflicted data the hydraulic properties of the soil was identified satisfactorily. There is only a small variance in the conductivity curve close to the saturated phase, but this is a well-known (unphysical) problem of the van Genuchten parametrization.

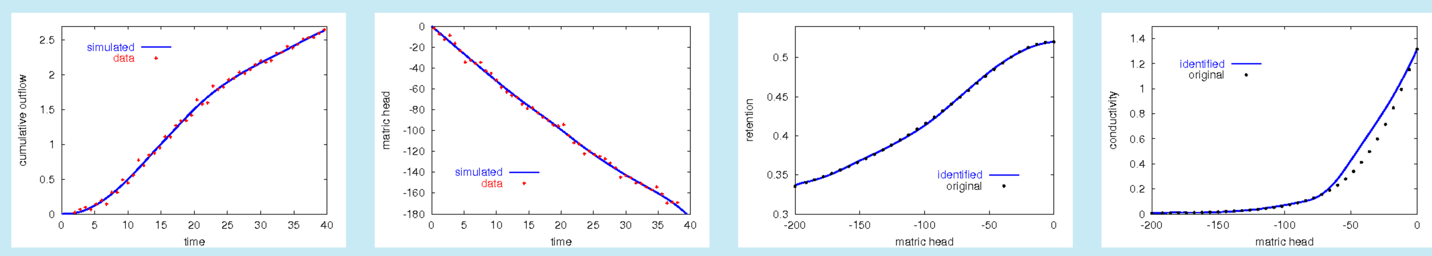

Figure 3: Formfree identification of the hydraulic properties

2) S. Bitterlich. *Identifizierung der hydraulischen Funktionen poröser Medien unter Verwendung formfreier Ansätze*, Dissertation, Universität Erlangen, 2003.

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