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Parameter estimation and accuracy matching strategies for 2-D reactor models

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Abstract

The mathematical modelling of a special modular catalytic reactor kit leads to a system of partial differential equation in two space dimensions. As customary, this model contains uncertain physical parameters, which may be adapted to fit experimental data. To solve this nonlinear least-squares problem we apply a damped Gauss–Newton method. A method of lines approach is used to evaluate the associated model equations. By an a priori spatial discretization, a large DAE system is derived and integrated with an adaptive, linearly implicit extrapolation method. For sensitivity evaluation we apply an internal numerical differentiation technique, which reuses linear algebra information from the model integration. In order not to interfere with the control of the Gauss–Newton iteration these computations are done usually very accurately and, therefore, with substantial cost. To overcome this difficulty, we discuss several accuracy adaptation strategies, e.g., a master–slave mode. Finally, we present some numerical experiments.

Keywords: Parameter estimation; Accuracy matching; Method of lines; Differential-algebraic systems; Extrapolation methods; Catalytic reactor models

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1. Introduction

Many chemical substances are produced by catalytic processes. For process development and optimization, the simulation of associated mathematical models is a helpful tool. Usually, within these models there are parameters whose exact values are not known. A common way of determining these values is parameter identification with nonlinear least-squares techniques.

We consider a two-dimensional, time-dependent model for a cylindrical reactor module, which is part of a special modular catalytic reactor kit [3]. This kit consists of standardised flange mounted reactor modules with different geometrical and thermal properties. This allows a simple realisation of a spectrum of reactor structures. A measurement module allows placing sensors at nearly any requested position inside the catalyst section of the reaction module.

In order to carry out parameter estimation for different models of the main reactor module, we combine, and slightly modify, efficient and robust algorithms for simulation [9,10] and sensitivity analysis [19] with a sophisticated, affine-invariant Gauss–Newton (GN) algorithm, which has proven to work very reliably in complex parameter identification problems, see, e.g., [5,16]. For an overview on state of the art techniques for parameter estimation in ordinary and partial differential equation models we refer, e.g., to the recent monograph [18] and references therein.

In the next section we first briefly describe our modelling of the basic reaction module. Then we briefly explain our method of lines treatment which yields a large ODE model. In Section 3 we present the numerical methods for the evaluation of the objective function of the GN-method (simulation), its derivative (sensitivity) computation, and finally, the damped GN-method. In Section 4 we discuss the problem of accuracy matching and propose a smoothness oriented matching strategy. In Section 5 some numerical examples are presented. We end with a short conclusion and an outlook on future work.

2. Mathematical model

The mathematical model for the interior of the catalytic reaction module is based on the usual balance equations for mass and energy using standard transport models. Mixing processes are included with a dispersion model. As a heat balance equation for the interior temperature T of the module we use

$$[\rho c_p \varepsilon + \rho^P c_p^P (1-\varepsilon)]\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(\lambda_z \frac{\partial T}{\partial z}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\lambda_r \frac{\partial T}{\partial r}\right) - \rho c_p w \frac{\partial T}{\partial z} + r_{\text{eff}}(-\Delta H). \tag{1}$$

The balances for the mass fractions g_i are expressed by

$$\frac{\partial g_i}{\partial t} = \frac{\partial}{\partial z}\left(D_z \frac{\partial g_i}{\partial z}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r D_r \frac{\partial g_i}{\partial r}\right) - w\frac{\partial g_i}{\partial z} + \frac{M_i}{\rho} v_{ij} r_{\text{eff}}. \tag{2}$$

The state equations for the wall model include axial heat conduction and convection and heat capacity of the reactor jacket and the fluid. Interior temperature at the wall (T_{R}) and temperature of the wall (T_{W}) are coupled by the transport equation

$$\lambda_r \partial T_{\text{R}}/\partial r = \alpha_{\text{W}}(T_{\text{R}} - T_{\text{W}}). \tag{3}$$

Otherwise the usual boundary conditions are applied, i.e., at $z = 0$: $T = T_{\mathrm{In}}(t, r)$, $g_i = g_{i,In}(t, r)$, and at $z = L$, as well as at $r = 0$, $r = R$, homogeneous Neumann conditions are prescribed. A detailed discussion of Eqs. (1–2) and an overview of heterogeneous gas catalytic modelling can be found in [1,2].

In order to solve the model equations we apply a classical MOL approach. In a first step, all spatial derivatives of the model are replaced by centred, 2nd-order finite difference approximations on appropriately chosen nonuniform tensor product grids. In order to avoid numerical oscillations for strongly convective systems, we add an appropriately chosen artificial diffusion term to Eqs. (1–2). After spatial discretization a very large system of differential-algebraic equations (DAE) arises, which may be written in the form

$$B(y; p)\dot{y} = f(y; p), \quad y(t_0) = y_0, \tag{4}$$

where $y(t)$ denotes the solution vector of dimension n at all spatial discretization points (z_l, r_k), and p is the vector of dimension q of parameters to be identified. Let n_z and n_r denote the number of grid points used for the spatial discretization of the cylindrical coordinate system. Let n_{PDE} denote the dimension of the system under consideration (temperature and mass fractions of the chemical species). The dimension of our semi-discrete system (4) is then given by $n = n_z \times n_r \times n_{\mathrm{PDE}}$. B is a possibly singular diagonal matrix and f a general nonlinear mapping. Both functions may depend also explicitly on the spatial coordinates (z, r) and time t. For ease of presentation we drop the latter dependencies in our notation.

3. Numerical treatment

3.1. Simulation

System (4) is nonlinear, stiff and block structured. For integration, we apply the linearly implicit extrapolation code LIMEX [9,10]. It uses as an elementary step the discretization

$$(B(y_0) - hA)(y_{k+1} - y_k) = hf(y_k) - (B(y_k) - B(y_0))(y_k - y_{k-1}), \tag{5}$$

where $A \approx (\partial/\partial y)(f - B\dot{y})|_{t=t_0}$ is the (approximate) Jacobian of the residual of (4) evaluated at a time point $t_0 \leqslant t_k$.

Combined with extrapolation this one-step method permits an adaptive stepsize and order control; for details see [6]. Applied to the discretized PDE-problem 4 the main amount of work for one step is the solution of the corresponding linear equations. The associated matrix $(B - hA)$ is very large, but sparse matrix techniques, direct or iterative, can be used for the solution of the linear system.

3.2. Sensitivity computation

Our parameter identification procedure requires the computation of the sensitivity matrix $S(t) := \mathrm{d}y(t)/\mathrm{d}p$. There are several well established ways to approximate $S(t)$, see, e.g., [14]. One approach is the differentiation of the DAE (4) with respect to p, yielding the q sensitivity equations for $S = [s_1 | \ldots | s_q]$,

$$\begin{aligned} B(y; p)\dot{s}_i &= \frac{\mathrm{d}}{\mathrm{d}p} f(y; p) - \frac{\mathrm{d}}{\mathrm{d}p} B(y; p)\dot{y} \\ &= f_y(y; p)s_i + f_p(y; p) - (B_y(y; p)s_i + B_p(y; p))\dot{y}. \end{aligned} \tag{6}$$

These equations are then solved simultaneously with the original equation. Applying LIMEX to this coupled system yields an associated Jacobian matrix **A**, which turns out to be

$$\mathbf{A} = \begin{pmatrix} A & & & \\ A_1 & A & & \\ \vdots & & \ddots & \\ A_q & & & A \end{pmatrix}, \tag{7}$$

where $A \approx (\partial/\partial y)(f - B\dot{y})|_{t=t_0}$, and $A_i \approx (\partial/\partial y)[f_y s_i + f_p - (B_y s_i + B_p)\dot{y}]|_{t=t_0}$. An integration of the coupled system using the matrix **A** would be rather expensive. However, replacing **A** by its block diagonal part, i.e., $\mathbf{A} \to \hat{\mathbf{A}} = \mathrm{diag}(A, \ldots, A)$ would speed up linear algebra computation dramatically. Therefore, this simplification is widely used, see, e.g., [15,19].

The major drawback of this approach is the need for explicitly given functions $f_y(t, y)$ and $f_p(t, y)$ in the case of constant B, and, additionally, $B_y(t, y)$ and $B_p(t, y)$ in the general case.

To overcome this problem, we replace, in part, the differentiation $\mathrm{d}/\mathrm{d}p$ in Eq. (6) by a finite difference approximation and get as sensitivity equations

$$B(y; p)\dot{s}_i = \frac{1}{\Delta p}\{f(y + \Delta p\, s_i; p + \Delta p) - f(y; p) - (B(y + \Delta p\, s_i; p + \Delta p) - B(y; p))\dot{y}\}. \tag{8}$$

Choosing $\Delta p = \sqrt{\mathrm{epmach}}$ (epmach = relative machine precision) and integrating with a prescribed tolerance tol, the precision of the sensitivity matrix $S(t)$ will be of order $\mathrm{tol} + \sqrt{\mathrm{epmach}}$, cf. [14]. For a wide range of problems this sensitivity computation turns out to be very efficient and robust [17].

3.3. Parameter identification

Assume that for some components of the state vector $y(z, r, t; p)$ measurements are available at some spatial points (z_ψ, r_ψ), $\psi = 1, \ldots, \Psi_\theta$, at times t_θ, $\theta = 1, \ldots, \Theta$. We arrange them in a vector y^{obs} of dimension m. In order to allow an unconstrained adaptation of temporal and spatial stepsizes (either automatically or by hand) the measurement points and times should be not necessarily part of their computational counterparts. Therefore, we need a proper interpolation procedure to generate solution approximations at the spatio-temporal measurement grid. For interpolation in time we use the global solution representation of LIMEX. Spatial interpolation is done by means of a monotone piecewise cubic hermite interpolation due to [12].

Having obtained with this procedure simulated counterparts y^{sim} for all components of the vector y^{obs} we can calculate a weighted residual vector

$$F(p) = \sum_{i=1}^{m} \frac{y_i^{\mathrm{sim}} - y_i^{\mathrm{obs}}}{y_i^w}. \tag{9}$$

To determine q uncertain parameters $p = (p_1, \ldots, p_q)^{\mathrm{T}}$ of the model equations one may solve the nonlinear least-squares problem

$$1/2\|F(p)\|_2^2 = 1/2F^{\mathrm{T}}F = \min. \tag{10}$$

A well established scheme for solving nonlinear least-square problems is the Gauss–Newton method. For the so-called small residual problems, the method is known to converge superlinearly near the solution

p^*. However, for bad initial guesses the method may diverge. To overcome this difficulty, several globalisation techniques exist, e.g., the popular Levenberg–Marquardt method. We use another way of enlarging the convergence domain, which is due to [8]. This method realizes a damped GN iteration, where the adaptive damping strategy and the convergence monitor are based on monitoring only GN corrections and not—as usual—the residuals. For a detailed mathematical derivation, analysis and comparison with other algorithms we refer to the upcoming textbook [7]. Omitting details, the main algorithmic flow of the method is sketched in the following informal algorithm.

Damped Gauss–Newton algorithm

p_0, λ_0 given
do $k = 0, \ldots, k_{\max}$
  $\Delta p_k = -J^+(p_k)F(p_k)$
$(*)\ p_{k+1} = p_k + \lambda_k \Delta p_k$
  $\overline{\Delta p}_{k+1} = -J^+(p_k)F(p_{k+1})$
  if $\|\overline{\Delta p}_{k+1}\| < \|\Delta p_k\|$ then

$$\lambda_{k+1} = \lambda_{k+1}^{\text{prio}} = \min\left(1, \frac{\|\Delta p_{k-1}\|}{\|\overline{\Delta p}_k - \Delta p_k\|}\lambda_k\right) \tag{11}$$

  else

$$\lambda_k = \lambda_k^{\text{post}} = \min\left(1, \frac{\lambda_k^2\|\Delta p_{k-1}\|^2}{2\|\overline{\Delta p}_{k+1} - (1-\lambda_k)\Delta p_k\|\Delta p_k\|}\right)$$

    goto $(*)$
  endif
  if $\|\overline{\Delta p}_{k-1}\| \leqslant \varepsilon_{GN}$ break
enddo

Herein, J^+ denotes the Moore–Penrose pseudoinverse of the Jacobian $J(p) = F'(p)$, $\overline{\Delta p}_k$ is the so-called simplified Gauss–Newton correction, λ_k^{prio} and λ_k^{post} are the a priori and a posteriori estimates for the optimal damping factor. The required tolerance is ε_{GN}.

In order to perform one iteration step, the main computational work is the evaluation of the GN–Jacobian J_k, which requires the computation of the sensitivity matrix S. To calculate the corrections Δp_k and $\overline{\Delta p}_{k+1}$ two linear least-square problems are solved by means of an QR-algorithm. If the monotonicity test

$$\|\overline{\Delta p}_{k+1}\| < \|\Delta p_k\| \tag{12}$$

is passed for the first trial iterate p_{k+1} just one function evaluation $F(p_{k+1})$ is required per step as this information is reused in the next iteration step. If the monotonicity test fails, the damping factor is reduced, and an additional function evaluation F_{k+1} for a new trial value p_{k+1} is computed. If the iteration converges to a solution p^* the usual linearized statistical analysis is done, see, e.g., [5], in order to get information on the statistical quality of the solution in terms of standard deviations and confidence intervals.

3.4. Accuracy matching

A sophisticated least-squares solver like [10] requires a certain smoothness of the underlying problem. In our case, the theoretical derivation requires that $F(p)$ is twice continuously differentiable. So, even

if F is an explicitely given function, the finite machine precision destroys this property formally, but for practical computations this roundoff error can be neglected. However, if F is a discretized operator, then rather large errors δF may show up. In general, as long as the temporal and spatial discretization remains fixed, not only the true operator, say $\hat{F}(p)$, but also the error δF depends smoothly on p. Thus, the discretized operator $F = \hat{F} + \delta F$ will vary smoothly with p also. However, changing a temporal and/or spatial stepsize while computing, e.g., $F(p_k)$ and $F(p_{k+1})$, will introduce a certain roughness into $F(p)$, as the assumption $\delta F(p_k) \approx \delta F(p_{k+1})$ is no longer valid. As a first consequence, the monotonicity test (12) may give wrong answers, and, furthermore, the evaluation of the a priori and a posteriori damping factors may be corrupted.

To overcome these difficulties, one may evaluate the discretized function $F(p)$ and its derivative $J(p) = F'(p)$ very accurately in order to mimic a smooth behaviour of F and J. Typical required tolerances for F-evaluation, ε_F, and J-evaluation, ε_J, are in the range $[10^{-4}, 10^{-7}]$. But, using such stringent accuracy requirements may be prohibitive for 2D time-dependent problems. So, one way to reduce the computational work is an adaptation of the tolerance with the following general strategy: relaxed accuracy requirement far from the solution and successively more stringent tolerances when approaching the solution of the parameter estimation problem. First steps in this direction have been made for damped Gauss–Newton schemes, combined with ODE models, in [5,16]. However, it turns out that the adaptation procedures must work very carefully in order not to disturb the GN-iteration severely. The main problem of such adaptation strategies is still the introduction of roughness into the objective function $F(p)$.

So, we propose an adaptation strategy which is smoothness oriented. First of all, we do not adapt the mathematical grid, either within one time integration or within the course of the GN-iteration. Instead, we use an initially chosen grid, which, however, may be nonuniform. Concerning the time stepping procedure of LIMEX, we use the idea of a master/slave integration which works as follows.

In order to meet a prescribed time tolerance ε_F^t, the very first GN function evaluation, $F(p_0)$, is done with the adaptive stepsize and order control switched on (master mode). All subsequent function and sensitivity evaluations are performed in slave mode, i.e., using the stepsizes, orders and, if necessary, the number of linear system iterations, of the master mode integration. During the slave mode integration for F, the error estimator of LIMEX is activated and the maximum value over time is recorded. If this achieved precision, say $\tilde{\varepsilon}_F^t$ is much larger than the prescribed precision of the master run, e.g.,

$$\tilde{\varepsilon}_F^t > \sigma_1 \varepsilon_F^t \ (\sigma_1 \approx 10) \tag{13}$$

this integration is repeated. Now again in master mode with ε_F^t as required tolerance.

In addition, a heuristical approach for checking the quality of the proposed damping factors has shown to improve the GN-iteration considerably. If within one step, say from k to $k+1$ the achieved error $\tilde{\varepsilon}_F^t(k+1)$ increases too much, i.e.,

$$\tilde{\varepsilon}_F^t(k+1) > \sigma_2 \tilde{\varepsilon}_F^t(k) \ (\sigma_2 \approx 10), \tag{14}$$

the current damping factor is not accepted and is reduced heuristically, e.g., by a factor of two. The subsequent re-evaluation of F is done still in slave mode.

For the spatial discretization a rather coarse tensor product grid $Z \otimes R$ is used. With that, the overall computing time for the GN-iteration is drastically reduced and the performance of the numerically disturbed iteration is rather close to the "optimal" performance, i.e., an iteration without discretization errors.

However, convergence will not occur to the true solution (of the continuous problem), but to a value which is corrupted by comparatively large temporal and spatial discretization errors. We try to estimate these errors (at least the order of magnitude) in the parameter estimates (not in the numerical solution $y^{\mathrm{sim}}(p^*)$) by the following refinement procedure.

Starting with $\mathrm{eps}_F^t(1) = \mathrm{eps}_F^t$, $Z(1) = Z$ and $R(1) = R$ we refine separately the time tolerance and initial grid sizes and perform in each case a full GN-iteration. Starting with the available solution $p_{111}^* = p^*(\mathrm{eps}_F^t(1), Z(1), R(1))$ as a very good initial guess, just one or two iteration steps are required. As a rough error estimate for p_{111}^* due to time discretization we use the differences $\|p^*(\mathrm{eps}_F^t(1), Z(1), R(1)) - p^*(\mathrm{eps}_F^t(2), Z(1), R(1))\| = \|p_{111}^* - p_{211}^*\|$. If the error estimate is of the order of the statistical error of the parameters the refinement is stopped, otherwise we continue the refinement process in order to get the estimate $\|p_{211}^* - p_{311}^*\|$ (and so forth, if necessary). Similarly the error due to spatial discretization in the z-direction and r-direction, respectively, are estimated.

This procedure is finished with a final Gauss–Newton iteration using appropriately refined tolerances and grids, i.e., for which the error estimates are in the range of the statistical error.

4. Numerical examples

We present some numerical experiments for our parameter identification procedure, applied to a heat transfer problem and a carbon monoxide gas oxidation model.

4.1. Heat conduction problem

To study heat transfer properties of our reactor module, we investigate a heat conduction problem without chemical reaction. A fixed bed blown by cold air will be heated up over a time period of several hours. The reactor allows temperature measurements at different radial and axial positions as well as in the reactor jacket. Smoothed measured temperature profiles were used to prescribe the boundary conditions at the inlet of the fixed bed and at the reactor walls. The measurements were realized for different tube diameters and flow rates, at a temperature range from 20 up to 350 °C. So, a spectrum of parameter estimation problems have been solved, using the data provided by [4]. The heat transport coefficients to be identified are the radial effective heat conduction λ_{r}, the wall heat transfer coefficient α_{w} of Eq. (3), and the width of a laminar flow film δ, cf. [13].

Concerning the numerical difficulty, the integration problem is rather easy to solve. No steep spatial gradients appear and there is a moderate dynamical behaviour in time. Using good starting values, the performance of the GN scheme is generally very robust and reliable—nearly independent of the applied accuracy matching strategy.

Things change, if we use rather bad initial guesses p_0. Comparing our new strategy with a standard approach where all F and J evaluations are done in master mode (for a fixed prescribed time tolerance) the new strategy allows the use of tolerances of $\varepsilon_F^t = 10^{-2}$, whereas the standard strategy requires values of about $\varepsilon_F^t = 10^{-4}$ in order to show a similar smooth behaviour as the new strategy. In all cases we use a grid of size $n_z \times n_r = 31 \times 16$. Our a posteriori error estimator for the accuracy of the parameters characterized this grid as sufficiently good for nearly all scenarios.

4.2. Carbon monoxide oxidation

The carbon monoxide oxidation reaction (CuO catalyst) [11] is prescribed by

$$\mathrm{CO} + \tfrac{1}{2}\,\mathrm{O_2} \Rightarrow \mathrm{CO_2}. \tag{15}$$

The effective reaction rate is determined by the mole fraction of the carbon monoxide and the Arrhenius function:

$$r_{\mathrm{eff}} = x_{\mathrm{CO}} k_\infty \exp\frac{-E_A}{RT}. \tag{16}$$

The specific enthalpy of the exothermal reaction is $\Delta H_R = -290 \times 10^3$ kJ/kmol. The mathematical model for this problem consists of a system of type (1–2) for temperature T and 3 chemical species. The dynamics of this system is dramatically more challenging than in the previous example. For slightly improperly chosen parameter values one can observe reactor runaway, as illustrated in Fig. 1. As local overheating (hot spots) causes catalyst damage, we stop the simulation whenever a temperature value $T > 650$ K is observed.

Real measurement data are available for the stationary state only. So, in order to study the effect of our temporal master/slave accuracy adaptation, we generate artificial measurement data for 50 spatial positions at 10 time points. To generate these data, we use parameter values close to the ones identified using the stationary data only. The artificial measurements are perturbed (relatively) using normally distributed random numbers with standard deviation $\sigma = 0.02$. Solution and measurement values for temperature and CO, in stationary state, are depicted in Fig. 2.

In our numerical experiments we try to re-identify the four diffusive parameters $\lambda_r = 0.8$, $\lambda_z = 0.18$, $D_r = 10^{-3}$, $D_z = 5 \times 10^{-6}$.

In the first step, we choose starting guesses p_0 for our GN method by a random selection, uniformly distributed in the cube $[p^{\mathrm{T}}/2, 2p^{\mathrm{T}}]$. About 20% of them turn out to be "too bad" in the sense, that the initial function evaluation $F(p_0)$ fails, i.e., was terminated by indicating reactor runaway. For about 30% of the test runs a smooth convergence of our GN scheme can be observed. A solution p^* is found typically within 5–6 GN iterations with at most 1–2 damped steps. The remaining test cases turn out to be very critical. The restart condition (13) and/or the reject condition (14) are activated at least one time, sometimes up to three times. Nevertheless, the highest GN-iteration count was 11 (successful) steps

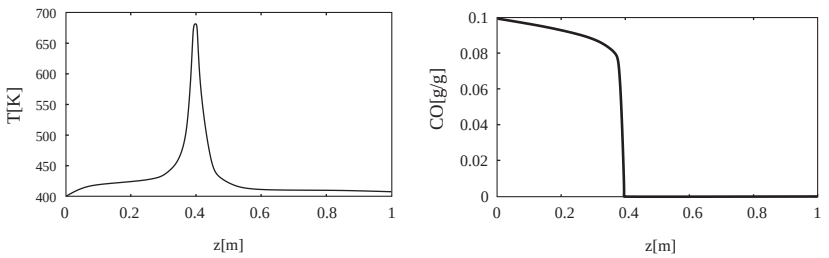

Fig. 1. Reactor runaway (temperature and CO concentration).

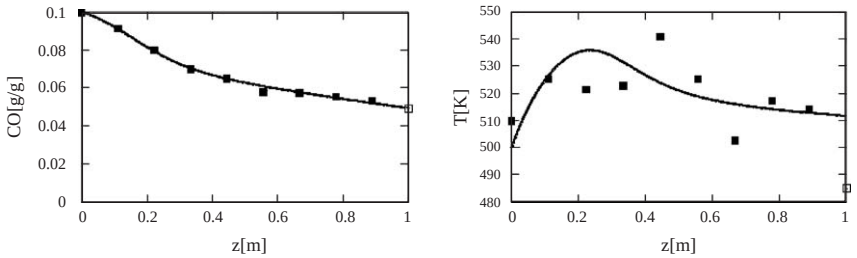

Fig. 2. Solution and measurement data for stationary state.

Table 1
Accuracy comparison of parameter estimates

Solution	λ_r	λ_z	D_r	D_z
Reference	0.708	0.181	0.995(−3)	0.479(−5)
Coarse	0.604	0.182	0.950(−3)	0.404(−5)
Refined	0.668	0.181	0.979(−3)	0.4590(−5)
Num. Err.	3%	1%	2%	4%
Stat. Err.	40%	1%	4%	8%

using 7 damped updates. Enlarging the cube leads to very similar results, except that for a certain sector of the cube the number of initial fail runs increases above average.

For all these test runs a fixed spatial grid $n_z \times n_r = 31 \times 16$ and an initial time tolerance of $\varepsilon_F^t = 10^{-2}$ was used.

In order to illustrate our a posteriori refinement procedure we have collected some results for one specific test run in Table 1. Generally, the coarse tolerance solution depends on the choice of p_0. However, the results given in Table 1 are quite representative.

In the first row of Table 1 a set of reference parameters, calculated on a very fine spatial grid, using a very stringent time tolerance, are given. Due to the measurement errors they differ from the values used to create the artificial measurements. In the second row the estimated parameters of the coarse grid/tolerance GN solution are given. The third row contains the values using the final GN solution with the automatically refined grid/tolerance values $n_z = 69$, $n_r = 36$, $\varepsilon_F^t = 0.25 \times 10^{-2}$. In our spatial refinement strategy we increase the number of uniformly distributed grid points by a factor of approximately $\sqrt{2}$, whereas the time tolerance is reduced by a factor of 2. The last two lines display the relative errors of this solution and the estimated relative error due to statistical uncertainty in terms of the individual confidence intervals. Obviously, the numerical errors are below the latter level. Computing numerically more accurate parameters would just waste computing time.

5. Conclusion and outlook

An adaptive accuracy matching strategy was developed, which enables a robust, reliable and efficient performance of a self-adaptive, damped Gauss–Newton scheme. Within the course of one GN-iteration

the temporal and spatial discretization is chosen initially and then frozen in order to have a discrete functional changing smoothly with changes in p. The nonlinear least-squares solution may be refined by repeated GN-iterations with varying, more accurate discretizations until a reasonable level of accuracy is reached, i.e., only slightly more accurate than the statistical uncertainty in the parameters to be estimated.

Further testing is required to check the quality of some of the heuristic parameters in our procedure. Furthermore, techniques for a locally oriented spatial refinement will be investigated. Based on error estimates for the numerical solution $y^{\mathrm{sim}}(p^*)$ one may try to insert new grid points in a nonuniform fashion.

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