Tutorial Overview of Dynamic Optimization and Advanced Control for Industrial Systems

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Abstract

Linear models are applied in many applications of industrial Advanced Process Control (APC) and a large user base of control engineers and consultants has grown to deploy and sustain these applications. Although project efficiency is increasing and implementation time is decreasing, there remains an art of applying linear Model Predictive Control (MPC) applications. This undocumented art is especially employed when the linear technology is extended to systems that have nonlinear characteristics. This paper describes methods to apply nonlinear models in adaptive model identification and control. This tutorial overview guides the user through a small multivariable level control problem that has a number of common characteristics to larger controllers seen in practice. The overview reveals additional fundamental capabilities by employing nonlinear models in applications of industrial relevance.

Keywords: advanced process control, differential algebraic equations, model predictive control, dynamic parameter estimation

1 1. Introduction

Applications of Model Predictive Control (MPC) are ubiquitous in a number 2 of industries such as refining and petrochemicals. Applications are also some-3 what common in chemicals, food manufacture, mining, and other manufacturing industries [1]. A majority of the applications employ linear models that are con-5 structed from empirical model identification, however, many of these processes have either semi-batch characteristics or nonlinear behavior. To ensure that the linear models are applicable over a wider range of operating conditions and disturbances, the linear models are retrofitted with elements that approximate 9 nonlinear control characteristics. Some of the nonlinear process is captured 10 by including gain scheduling, switching between multiple models depending on 11 operating conditions, and other logical programming when certain events or 12 conditions are present. The art of using linear models to perform nonlinear 13

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control has been refined by a number of control experts to extend linear MPC
to a wider range of applications. While this approach is beneficial in deploying
applications, maintenance costs are increased and sustainability is decreased
due to the complexity of the heuristic rules and configuration.

The purpose of this article is not to detail the best practices with linear 18 models, but instead to give practical guidance on using nonlinear models in the 19 typical steps of an MPC project. Recent advancements in numerical techniques 20 have permitted the direct application of nonlinear models in control applica-21 tions [2], however, many nonlinear MPC applications require advanced training 22 to build and sustain an application. Perhaps the one remaining obstacle to fur-23 ther utilization of nonlinear technology is the ease of deploying and sustaining 24 applications by practitioners. Up to this point, there remain few actual indus-25 trial applications of control based on nonlinear models. The objective of this 26 paper is to reduce the barriers to implementation of nonlinear advanced control 27 applications. This is attempted by giving a practical guide and providing details 28 29 on the following topics:

- nonlinear model development combining empirical and first principles el ements
- ³² parameter estimation from dynamic data
- advanced process control with large-scale nonlinear models
- conversion of differential equations into algebraic equations for efficient solution by nonlinear programming solvers

In addition to the theoretical underpinnings of the techniques, a practical 36 application with process data is used to demonstrate model identification and 37 control. The application used in this paper is a simple level control system that 38 was selected to illustrate the concepts without burdening the reader with model 39 complexity. In practice, much larger and more complex systems can be solved 40 using these techniques. An illustration of scale-up to larger problems gives an 41 indication of the size that can be solved with current computational resources. 42 The example problems are demonstrated with the APMonitor software, a freely 43 available package for solution of differential and algebraic equation (DAE) sys-44 tems. Specific examples are included in the appendices with commands to re-45 produce the examples in this paper. 46

This paper includes a number of innovative techniques for solving large-47 scale control and optimization problems. One novel contribution of this paper 48 is modified L_1 -norm objective forms for estimation and control. These objective 49 forms have a number of advantages over traditional squared-error or L_2 -norm 50 objectives that are often reported in the literature. Another contribution is 51 the tutorial nature of the article with concise source code that can be used to 52 reproduce the results or develop further applications. The target audience is 53 the practitioner or researcher interested in applying nonlinear estimation and 54 control to challenging applications of industrial relevance. 55

⁵⁶ 2. Model Identification with Nonlinear Equations

A critical aspect of any control project is reliable model identification. Linear 57 model identification used in practice is typically with Finite Impulse Response 58 (FIR) or State Space (SS) forms. Nonlinear model identification also involves 59 adjustment of parameters to fit process data. Linear model identification is 60 often an empirical approach while nonlinear models have some structure that 61 results from material and energy balances, reaction kinetic mechanisms, or other 62 pre-defined model structure. As a result of the model structure, there are fewer 63 parameters that need to be adjusted to fit the process response. Model struc-64 ture may also include constraints such as fixed gain ratios, zero lower limits on 65 compositions, or other bounds that reflect physical realism. 66

Along with model form, the form of the identification objective function is important to ensure desirable results. The most common objective form is the least squares form: $(y_{model} - y_{meas})^2$ (see Equation 1). Although intuitive and simple to implement, the squared error form has a number of challenges such as sensitivity to bad data or outliers. The sensitivity to outliers is exacerbated by the squared error objective, commonly proposed for dynamic data reconciliation [3] [4] [5] [6] [7].

Table 1 details the equations of the typical squared error norm and the novel 74 L_1 -norm objective. A new form of the identification objective improves some 75 of the problems with the L_2 form. The L_1 -norm formulation in Equation 2 is 76 less sensitive to data outliers and better rejects measurement noise. The form 77 is similar to an absolute value function but is instead solved with inequality 78 constraints and slack variables. The absolute value operator is not continuously 79 differentiable which can cause convergence problems for Nonlinear Programming 80 (NLP) solvers. On the other hand, the L_1 -norm slack variables and inequalities 81 create an objective function that is smooth and continuously differentiable. 82

Other challenges in aligning the model to measured values (data reconcili-83 ation) include lack of data diversity to obtain certain constants or co-linearity 84 of parameters. The sensitivity of parameters to the objective function can help 85 guide which parameters have a significant effect on the outcome [8]. One so-86 lution to automatically eliminate parameters with little sensitivity to objective 87 is to impose a small penalty on parameter movement from a nominal value 88 [9]. This approach automatically prevents unnecessary movement of parameter 89 values that have little effect on the results of the parameter estimation. Histor-90 ically, most of the techniques for parameter estimability rely on steady-state or 91 statistical analysis of linearized systems. The approach in this article extends 92 the linear or steady-state analysis to dynamic and nonlinear systems. 93

⁹⁴ 3. Application: Quadruple Tank Level Control

A quadruple tank process shown in Figure 1 has been the subject of theoretical [10] and practical demonstrations [11] [12] [13] [14] of a multivariable and highly coupled system [12]. The four tank process has also been a test application for application of decentralized and coordinated control techniques

Table 1: Estimation: Two Forms for Dynamic Data Reconciliation

Estimation with a Squared Error Objective (Most Common)

$$\min_{d} \Phi = (y_x - y_m)^T W_m (y_x - y_m) \dots + (\Delta d)^T c_{\Delta d}$$

$$\dots + (y_m - \hat{y}_m)^T W_p (y_m - \hat{y}_m)$$

s.t.
$$0 = f(\dot{x}, x, u, p, d)$$

$$0 = g(y_x, x, u, d)$$

$$a \ge h(x, u, d) \ge b$$
(1)

Estimation with an L_1 -norm Objective (Better Outlier Rejection)

$$\min_{d} \Phi = w_{m}^{T} (e_{U} - e_{L}) + w_{p}^{T} (c_{U} + c_{L}) + (\Delta d)^{T} c_{\Delta d}$$
s.t.
$$0 = f(\dot{x}, x, u, p, d)$$

$$0 = g(y_{x}, x, u, d)$$

$$a \ge h(x, u, d) \ge b$$

$$e_{U} \ge y_{x} - y_{U}$$

$$e_{L} \ge y_{L} - y_{x}$$

$$c_{U} \ge y_{x} - \hat{y}_{m}$$

$$c_{L} \ge \hat{y}_{m} - y_{x}$$

$$e_{U}, e_{L}, c_{U}, c_{L} \ge 0$$
(2)

Nomenclature for Equations 1 and 2 $\,$

Φ	objective function
y_x	measurements $(y_{s,0},\ldots,y_{s,n})_{T}^{T}$
y_m	model values $(y_{m,0},\ldots,y_{m,n})^T$
\hat{y}_m	prior model values $(\hat{y}_{m,0},\ldots,\hat{y}_{m,n})^T$
w_m, W_m	penalty outside measurement dead-band
w_p, W_p	penalty from the prior solution
$c_{\Delta d}$	penalty from the prior disturbance values
f	equation residuals
x	states
u	inputs
d	parameters or unmeasured disturbances
Δd	change in parameters
g	output function
h	inequality constraints
a	lower limits
b	upper limits
e_U	slack variable above the measurement dead-band
e_L	slack variable below the measurement dead-band
c_U	slack variable above the previous value
c_L	slack variable below the previous value

⁹⁹ [15] [16]. A number of other interesting characteristics of this process include ¹⁰⁰ configurations that cause the system to go unstable. This can be observed by ¹⁰¹ showing that there are right-hand plane (RHP) zeros. Another challenge is the ¹⁰² nonlinear tendency of the system. For example, this can be characterized by ¹⁰³ variable gains of the manipulated variables (MVs) to the controlled variables ¹⁰⁴ (CVs).

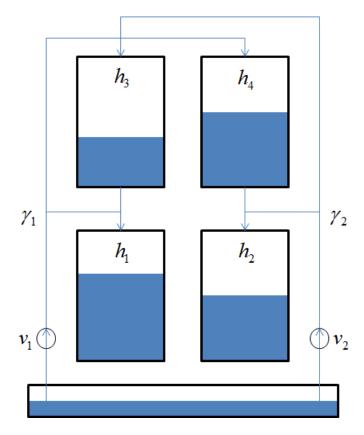


Figure 1: Diagram of the quadruple tank process. Pump 1 supplies tanks 1 and 4 while pump 2 supplies tanks 2 and 3.

The four tank process has two pumps that are adjusted with variable voltage 105 to pump 1 (v_1) and pump 2 (v_2)). A fraction of water from pump 1 is diverted 106 to tank 1 proportional to γ_1 and to tank 4 proportional to $(1 - \gamma_1)$. Similarly, 107 a fraction of water from pump 2 is diverted to tank 2 proportional to γ_2 and 108 to tank 3 proportional to $(1 - \gamma_2)$. The values that determine γ_1 and γ_2 are 109 manually adjusted previous to the experiment and are held constant through-110 out a particular period of data collection. All tanks are gravity drained and tank 111 3 outlet enters tank 1. Tank 4 outlet enters tank 2, creating a coupled system 112 of manipulated and controlled variables. For $(\gamma_1 + \gamma_2) \in (0, 1)$, the linearized 113

system has no RHP zeros with for $(\gamma_1 + \gamma_2) \in (1, 2)$, the linearized system has one RHP zero [10]. A RHP zero indicates that there may either be overshoot or an inverse response to a step change in the manipulated variable.

A combination of material balances and Bournoulli's law yields the process model for the four tank process as shown in Equation 3. The equations are also displayed in Appendix A in the APMonitor Modeling Language.

$$q_{a} = k_{m}v_{1} + k_{b}$$

$$q_{b} = k_{m}v_{2} + k_{b}$$

$$q_{1,in} = \gamma_{1}q_{a} + q_{3,out}$$

$$q_{2,in} = \gamma_{2}q_{b} + q_{4,out}$$

$$q_{3,in} = (1 - \gamma_{2}) q_{b}$$

$$q_{4,in} = (1 - \gamma_{1}) q_{a}$$

$$q_{1,out} = c_{1}\sqrt{2gh_{1}}$$

$$q_{2,out} = c_{2}\sqrt{2gh_{2}}$$

$$q_{3,out} = c_{3}\sqrt{2gh_{3}}$$

$$q_{4,out} = c_{4}\sqrt{2gh_{4}}$$

$$A_{1}\frac{\partial h_{1}}{\partial t} = q_{1,in} - q_{1_{o}ut}$$

$$A_{2}\frac{\partial h_{2}}{\partial t} = q_{2,in} - q_{2_{o}ut}$$

$$A_{3}\frac{\partial h_{3}}{\partial t} = q_{4,in} - q_{4_{o}ut}$$
(3)

120 where

121

	γ1	split factor for tanks 1 and 4
-	γ_2	split factor for tanks 2 and 3
(c_i	outflow factor for tank i
i	k_m	valve linearization slope
i	k_b	valve linearization intercept
(a	flow from pump 1
(Дь	flow from pump 2
($_{li,in}$	inlet flow to tank i
(li,out	outlet flow from tank i
_	A_i	cross-sectional area of tank i
j	h_i	height of liquid in tank i

The process model is nonlinear because the outlet flow is proportional to the square root of the liquid level. In this experiment, tanks 1 and 3 and tanks 2 and 4 have the same outlet diameter making $c_1 = c_3$ and $c_2 = c_4$. Additionally, tanks 1 and 3 have a cross-sectional area of $28cm^2$ while tanks 2 and 4 have a cross-sectional area of $32cm^2$. Unknown parameters include γ_1 , γ_2 , $c_{1,3}$, $c_{2,4}$, k_m , and k_b . The unknown parameters are determined from dynamic data.

¹²⁸ 3.1. Parameter Estimation from Dynamic Data

Pseudo-random binary signals (PRBS) are a popular technique to generate
linear plant response models from data [17]. This section demonstrates that
PRBS-generated data can be used to determine optimal parameters for nonlinear dynamic models as well. Another technique for fitting model parameters to

process data is the use of multiple steady-state data sets [18]. Control engineers 133 identify steady-state periods that cover the major process operating regions of 134 interest. One of the drawbacks to fitting a model with steady-state data is 135 that dynamic parameters cannot be fit from the data. Dynamic parameters 136 are those values that are multiplied by the derivatives with respect to time in 137 the equations. In the case of a linear first order system $\left(\tau \frac{\partial y}{\partial t} = -y + Ku\right)$ the 138 dynamic parameter is τ . However, process time constants can typically be es-139 timated from process fundamentals such as vessel holdups and flow rates. In 140 many cases, the time constants can be approximated reasonably well. However, 141 using only steady-state data for fitting parameters can limit the observability of 142 certain parameters that can only be determined with dynamic data. If nonlinear 143 MPC is to be used to the full potential, dynamic data must be used to fit the 144 models. 145

Using dynamic data to fit nonlinear dynamic models has a number of challenges. One of the challenges is that the data reconciliation problem can be very large. The data reconciliation problem is large because an instance of the model must be calculated at every time instant where a measurement is available. Using the simultaneous optimization of model and objective function, the number of model states at a particular time is multiplied by the number of time steps.

153 3.2. Quadruple Tank Parameter Estimation

For the quadruple tank process the model has only 14 differential or algebraic 154 states. When calculated over the PRBS data horizon the resulting optimiza-155 tion problem has 5766 to 11,526 variables, depending on the objective function 156 form. There are no differential states in the optimization problem due to the 157 orthogonal collocation transformation (see Section 5). Orthogonal collocation 158 on finite elements is one of the methods to convert DAE systems into a Nonlin-159 ear Programming (NLP) problem [19]. This is accomplished by approximating 160 time derivatives of the DAE system as algebraic relationships. Figure 2 shows 161 the results of the reconciliation to the PRBS-generated data. 162

Only levels for tanks 1 and 2 are measured as shown in Figure 2. For the 163 quadruple tank process 6 parameters were estimated, namely γ_1 , γ_2 , $c_{1,3}$, $c_{2,4}$, 164 k_m , and k_b . The optimization problem overview is shown in Table 2 while 165 initial and final values of the parameters are displayed in Table 3. An APM 166 MATLAB script for configuring and solving this problem is shown in Appendix 167 B. The MATLAB script uses the APMonitor Modeling Language [20] model (see 168 Appendix A) to create the differential and algebraic (DAE) model. APMonitor 169 translates the problem into an NLP and IPOPT, an interior point large-scale 170 nonlinear programming solver [21], is used to solve the resulting optimization 171 problem. A summary of the optimization problem and the solution is shown in 172 Table 2. 173

Using different objective function forms resulted in similar parameter estimates and comparable model predictions. As seen in Table 3, the optimal values for the parameters were well within the upper and lower constraints.

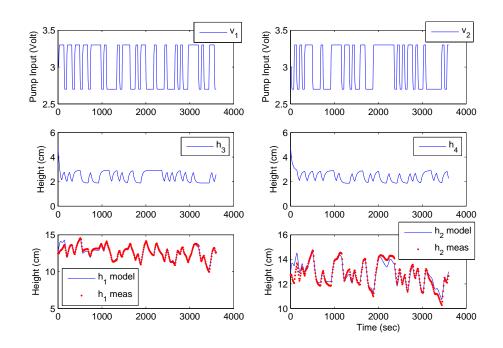


Figure 2: The results of the dynamic parameter estimation using PRBS generated data.

Optimization Problem Overview		
Description	L_1 -Norm	Squared
		Error
Iterations	33	10
CPU Time (2.5 GHz Intel i7 Processor)	32.5 sec	10.3 sec
Number of Variables	11,526	5,766
Number of Equations	11,520	5,760
Degrees of Freedom	6	6
Number of Jacobian Non-zeros	$40,\!312$	28,792

Table 2: Summary of the Dynamic Data Reconciliation

These constraints were set based on knowledge of the process; a violation of these constraints would indicate unreasonable parameter values. In this case, the L_1 -Norm optimization problem was roughly twice the size and required 3 times the amount of CPU time to find a solution. In this case, the increased computational time is additional cost associated with improved outlier rejection and parameter estimates.

Initial and Fir	al Values of	the Estimat	ion Problem		
Parameter	Initial	Lower	Upper	L_1 -Norm	Squared
	Value	Bound	Bound		Error
γ_1	0.43	0.20	0.80	0.627	0.585
γ_2	0.34	0.20	0.80	0.591	0.548
$c_{1,3}$	0.071	0.010	0.200	0.0592	0.0630
$c_{2,4}$	0.057	0.010	0.200	0.0548	0.0582
k_m	10.0	3.0	20.0	3.543	3.444
k_b	0.00	-2.00	2.00	-1.675	-0.810

Table 3: Results of the Dynamic Data Reconciliation

183 4. Nonlinear Control and Optimization

There are many challenges to application of Differential and Algebraic Equa-184 tions (DAEs) directly in nonlinear control and optimization. Enabling advances 185 include simultaneous methods [22], decomposition methods [23] [24], efficient 186 nonlinear programming solvers [21], improved estimation techniques [25] [26] [27] 187 [28], and experience with applications to industrial systems [9] [29]. In particu-188 lar, industrial applications require high service availability, reasonable extrapo-189 lation to operating conditions outside the original training set, and explanatory 190 tools that reveal the rationale of the optimization results. Other motivating 191 factors include consideration of lost opportunity during application develop-192 ment, sustainability of the solution, and ease of development and maintenance 193 by engineers without an advanced training. In many instances non-technical 194 challenges such as equipment and base-control relability, operator training, and 195 management support are critical factors in the success of an application [30]. 196

The most popular objective function form in academia and for industrial applications is the squared error or L_2 -norm objective (see Equation 4). In this form, there is a squared penalty for deviation from a setpoint or desired trajectory. The squared error objective is simple to implement, has a relatively intuitive solution, and is well suited for Quadratic Programming (QP) or Nonlinear Programming (NLP) solvers.

An alternative form of the objective function is the L_1 -norm objective (see Equation 5) that has a number of advantages over the squared error form similar to those discussed for the estimation case. For control problems, the advantage is not in rejection of outliers but in the explicit prioritization of control objectives. The L_1 -norm simultaneously optimizes multiple objectives in one optimization problem as the solver manipulates the degrees of freedom selectively for the objective function contributions that have the highest sensitivity. For problems that have safety, environmental, economic, and other competing priorities, the L_1 -norm gives the most intuitive form that manages these trade-offs. Table 4 details the square error and L_1 -norm objective functions.

213 4.1. Nonlinear Control of the Quadruple Tank System

Returning to the quadruple tank system, the squared error model parameters 214 from Section 3.2 are used to update the model. Either the squared-error or the 215 L_1 -norm objective estimation values can be used because of nearly equivalent 216 results. Data reconciliation can either be performed once or repeatedly as new 217 measurements arrive in a receding horizon approach. As new measurements 218 arrive, the model is readjusted to fit the data and continually refine the model 219 predictions. These updated parameters can then be used in the MPC application 220 to better predict the future response. 221

Once the model is updated, nonlinear control calculates the optimal trajec-222 tory of Manipulated Variables (MV). In this case, a future move plan of the 223 voltage to the two pumps is calculated and displayed Figure 3. MV moves are 224 constrained by change, upper, and lower limits. The change constraints are set 225 to limit the amount that the MV can move for each control action step and in 226 this case the move limit is set to $|\Delta MV| \leq 1$. With a cycle time of 1 second, 227 the rate that the voltage to the pump can change is $\pm 1 \frac{\dot{V}}{sec}$. The control action 228 is also constrained by absolute minimum $(MV_L = 1)$ and maximum $(MV_U = 6)$ 229 limits. The lower limit is reached for the first pump (v1) and remains at the 230 lower limit for 30 seconds before settling at the steady state value at 1.41V. 231 The upper limit is reached for second pump (v2) within two steps into the hori-232 zon and afterwards settles to a steady state value of 4.58V. This over-shoot 233 or under-shoot of manipulated variables is typical for controlled variable (CV) 234 tuning that is faster than the natural process time constant. The natural pro-235 cess time constant is the speed of response due to a step change in a process 236 input. When requesting a response that is faster than this nominal step change, 237 the manipulated variables must over-react to move the process faster. In most 238 cases, steady state values of the manipulated variables are independent of the 239 controller tuning. 240

CV tuning is a critical element to achieving desirable control performance.
Aggressive CV tuning is shown in this example, giving over- or under-shoot of
the manipulated variables. For CV tuning that is equal to the natural process
time constant, there will typically be a step to the new solution. For slower CV
tuning, the MV ramps to the steady state value.

There are many types of CV tuning options that are typical in linear or nonlinear control applications. In this case, an L_1 -norm with dead-band is demonstrated for the simulated controller. The speed of the CV response is dictated by an upper and lower first order reference trajectory with time constant τ_c . Only values that are outside this dead-band are penalized in the objective

Table 4: Control: Two Objective Forms for Nonlinear Model Predictive Control

Control Squared Error Objective

$$\min_{u} \Phi = (y_m - y_t)^T W_t (y_m - y_t) \dots$$

$$\dots + (y_m)^T c_y + (u)^T c_u + (\Delta u)^T c_{\Delta u}$$

s.t.
$$0 = f(\dot{x}, x, u, p, d)$$

$$0 = g(y_x, x, u, d)$$

$$a \ge h(x, u, d) \ge b$$
(4)

Control L_1 -norm Objective

$$\min_{d} \Phi = w_{hi}^{T} (e_{hi}) + w_{lo}^{T} (e_{lo}) \dots \\
\dots + (y_{m})^{T} c_{y} + (u)^{T} c_{u} + (\Delta u)^{T} c_{\Delta u} \\
\text{s.t.} \quad 0 = f(\dot{x}, x, u, p, d) \\
0 = g(y_{x}, x, u, d) \\
a \ge h(x, u, d) \ge b \\
\tau_{c} \frac{\partial y_{t,hi}}{\partial t} + y_{t,hi} = sp_{hi} \\
\tau_{c} \frac{\partial y_{t,lo}}{\partial t} + y_{t,lo} = sp_{lo} \\
e_{hi} \ge (y_{m} - y_{t,hi}) \\
e_{lo} \ge (y_{t,lo} - y_{m})
\end{cases}$$
(5)

Nomenclature for Equations 4 and 5

Φ	objective function
y_m	model values $(y_{m,0},\ldots,y_{m,n})^T$
$y_{t,hi}, y_{t,lo}$	desired trajectory dead-band
w_{hi}, w_{lo}	penalty outside trajectory dead-band
$c_y, c_u,$	cost of y , u and Δu , respectively
$c_{\Delta u}$	
f	equation residuals
x	states
u	inputs
d	parameters or unmeasured disturbances
g	output function
h	inequality constraints
a	lower limits
b	upper limits
au	time constant of desired controlled variable re-
	sponse
e_{lo}	slack variable below the trajectory dead-band
e_{hi}	slack variable above the trajectory dead-band

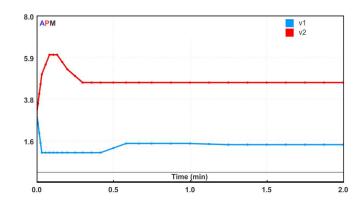


Figure 3: Optimal solution of the voltage input to the pumps 1 and 2.

²⁵¹ function. The form of this controller objective is desirable for minimizing unnecessary MV movement to achieve a controller objective. In this form, MV ²⁵³ movement only occurs if the projected CV response is forecast to deviate from ²⁵⁴ a pre-described range. Figures 4 and 5 display the CV response along with the ²⁵⁵ upper and lower trajectories that define the control objective.

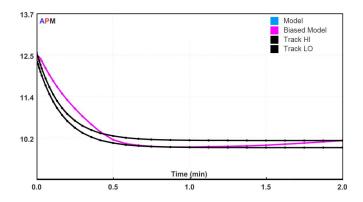


Figure 4: Height response in tank 1 and the associated controller objective.

²⁵⁶ 5. Numerical Solution of DAE Systems

The simultaneous solution of the model equations and objective function has a number of advantages over other techniques. Other methods include the direct shooting approaches [31] where the objective function and model equations are solved separately and iteratively towards an optimal solution. With a simultaneous solution of the objective and model equations, there is improved

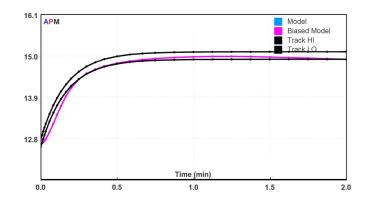


Figure 5: Height response in tank 2 and the associated controller objective.

computational performance with additional degrees of freedom. Another advantage with a simultaneous solution is that a general DAE model form can be
posed in open equation format (see Equation 6).

$$0 = f\left(\frac{\partial x}{\partial t}, x, y, p, d, u\right)$$

$$0 = g(x, y, p, d, u)$$

$$0 \le h(x, y, p, d, u)$$
(6)

In open equation format, DAE models of index-1 or higher are solved without 265 266 rearrangement. The solution of Equation 6 is determined by the initial state x_0 , a set of parameters p, a trajectory of disturbance values $d = (d_0, d_1, \dots, d_{n-1})$, 267 and a sequence of control moves $u = (u_0, u_1, \ldots, u_{n-1})$. The values of the pa-268 rameters, disturbances, or decision variables (p, d, and u) are discrete values 269 over the time horizon to make the problem tractable for numerical solution (e.g. 270 Manipulated Variables in Figure 6). On the other hand, integrated variables are 271 determined from differential and algebraic equations and generally have a con-272 tinuous profile (e.g. Controlled Variables in Figure 6). One solution approach to 273 this dynamic system is the conversion of the DAE system to algebraic equations 274 through direct transcription [2]. This technique is also known as orthogonal 275 collocation on finite elements [32]. Converting the DAE system to a Nonlinear 276 Programming (NLP) problem permits the solution by large-scale solvers [4] [33]. 277 Additional details of the simultaneous approach are shown in Section 5.1 and 278 an example problem in Section 5.2. 279

280 5.1. Derivation of Weighting Matrices for Orthogonal Collocation

The objective is to determine a matrix M that relates the derivatives to the non-derivative values over a horizon at points $1, \ldots, n$. In this case, four points are shown for the derivation. The initial value, x_0 , is a fixed initial condition.

$$\begin{bmatrix} \dot{x}_1\\ \dot{x}_2\\ \dot{x}_3 \end{bmatrix} = M \left(\begin{bmatrix} x_1\\ x_2\\ x_3 \end{bmatrix} - \begin{bmatrix} x_0\\ x_0\\ x_0 \end{bmatrix} \right)$$
(7)

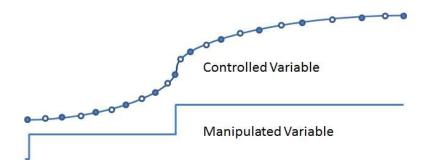


Figure 6: Dynamic equations are discretized over a time horizon and solved simultaneously. The solid nodes depict starting and ending locations for local polynomial approximations that are pieced together over the time horizon. With one internal node for each segment, this example uses a 2nd order polynomial approximation for each step.

The solution of the differential equations at discrete time points is approximated by a Lagrange interpolating polynomial as shown in Equation 8.

$$x(t) = A + Bt + Ct^2 + Dt^3 \tag{8}$$

Time points for each interval are chosen according to Lobatto quadrature. All 286 time points are shifted to a reference time of zero $(t_0 = 0)$ and a final time of 287 $t_n = 1$. For 3 nodes per horizon step, the one internal node is chosen at $t_1 = \frac{1}{2}$. 288 An example of internal nodes are displayed in Figure 6 where the horizon is 289 broken into multiple intervals of Lobatto quadrature with 3 nodes per horizon 290 step (one internal node). In the case of 4 nodes per horizon step, the internal 291 values are chosen at $t_1 = \frac{1}{2} - \frac{\sqrt{5}}{10}$ and $t_2 = \frac{1}{2} + \frac{\sqrt{5}}{10}$. With 5 nodes, time values are 292 $\frac{1}{2} - \frac{\sqrt{21}}{14}$, $\frac{1}{2}$, and $\frac{1}{2} + \frac{\sqrt{21}}{14}$. At 6 nodes, time values are $\frac{1}{2} - \frac{\sqrt{7+2\sqrt{7}}}{42}$, $\frac{1}{2} - \frac{\sqrt{7-2\sqrt{7}}}{42}$, $\frac{1}{2} - \frac{\sqrt{7-2\sqrt{7}}}{42}$, $\frac{1}{2} + \frac{\sqrt{7-2\sqrt{7}}}{42}$, and $\frac{1}{2} + \frac{\sqrt{7+2\sqrt{7}}}{42}$. In this derivation, a third-order polynomial approximates the solution at the four points in the horizon. Increasing the 293 294 295 number of collocation points increases the corresponding polynomial order. For 296 initial value problems, the coefficient A is equal to x_0 , when the initial time is 297 arbitrarily defined as zero. To determine the coefficients B, C, and D, Equation 298 8 is differentiated and substituted into Equation 7 to give Equation 9. Note that 299 the A coefficient from Equation 8 is cancelled by x_0 on the right-hand side of 300 301 Equation 9.

$$\begin{bmatrix} B + 2Ct_1 + 3Dt_1^2 \\ B + 2Ct_2 + 3Dt_2^2 \\ B + 2Ct_3 + 3Dt_3^2 \end{bmatrix} = M \begin{bmatrix} Bt + Ct_1^2 + Dt_1^3 \\ Bt + Ct_2^2 + Dt_3^3 \\ Bt + Ct_3^2 + Dt_3^3 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2t_1 & 3t_1^2 \\ 1 & 2t_2 & 3t_2^2 \\ 1 & 2t_3 & 3t_3^2 \end{bmatrix} \begin{bmatrix} B \\ C \\ D \end{bmatrix} = M \begin{bmatrix} t_1 & t_1^2 & t_1^3 \\ t_2 & t_2^2 & t_3^2 \\ t_3 & t_3^2 & t_3^3 \end{bmatrix} \begin{bmatrix} B \\ C \\ D \end{bmatrix}$$

$$(9)$$

³⁰² Finally, rearranging and solving for M gives the solution shown in Equation 10.

$$M = \begin{bmatrix} 1 & 2t_1 & 3t_1^2 \\ 1 & 2t_2 & 3t_2^2 \\ 1 & 2t_3 & 3t_3^2 \end{bmatrix} \begin{bmatrix} t_1 & t_1^2 & t_1^3 \\ t_2 & t_2^2 & t_2^3 \\ t_3 & t_3^2 & t_3^3 \end{bmatrix}^{-1}$$
(10)

The final form that is implemented in practice is shown in Equation 11 by inverting M and factoring out the final time t_n $(t_n N = M^{-1})$). This form improves the numerical characteristics of the solution, especially as the time step approaches zero $(t_n \to 0)$.

$$t_n N \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} - \begin{bmatrix} x_0 \\ x_0 \\ x_0 \end{bmatrix} \right)$$
(11)

The matrices that relate $\frac{\partial x}{\partial t}$ to x are given in Table 5 for intervals with 3 to 6 nodes.

³⁰⁹ 5.2. Example Solution by Orthogonal Collocation

A simultaneous solution demonstrates the application of orthogonal collocation. In this case, the first order system $\tau \frac{\partial x}{\partial t} = -x$ is solved at 6 points from $t_0 = 0$ to $t_n = 10$ using Equation 18. In this case $\tau = 5$ and the initial condition is specified at $x_0 = 1$. For this problem, the time points for $\frac{\partial x}{\partial t}$ and x are selected as 0, 1.175, 3.574, 6.426, 8.825, and 10. The value of x is specified at $t_0 = 0$ due to the initial condition. As a first step, equations for $\frac{\partial x}{\partial t}$ are generated in Equation 20.

$$\frac{\partial x}{\partial t} = \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \\ \dot{x}_5 \end{bmatrix} = (t_n N_{5x5})^{-1} \left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} - \begin{bmatrix} x_0 \\ x_0 \\ x_0 \\ x_0 \\ x_0 \\ x_0 \end{bmatrix} \right)$$
(20)

Substitution of Equation 20 into the derivatives of the model equation yields a linear system of equations as shown in Equation 21.

$$\tau \frac{\partial x}{\partial t} = -x$$

$$\tau (t_n N_{5x5})^{-1} \left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} - \begin{bmatrix} x_0 \\ x_0 \\ x_0 \\ x_0 \\ x_0 \end{bmatrix} \right) = - \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix}$$

$$(21)$$

Equation 21 is rearranged and solved with a linear algebra as shown in Equation 22.

Table 5: Orthogonal Collocation on Finite Elements
Orthogonal Collocation Matrices

$$t_n N_{2x2} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} x_0 \\ x_0 \end{bmatrix} \right) \quad (12) \qquad N_{2x2} = \begin{bmatrix} 0.75 & -0.25 \\ 1.00 & 0.00 \end{bmatrix} \quad (13)$$
$$t_n N_{3x3} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} - \begin{bmatrix} x_0 \\ x_0 \\ x_0 \end{bmatrix} \right) \qquad N_{3x3} = \begin{bmatrix} 0.436 & -0.281 & 0.121 \\ 0.614 & 0.064 & 0.046 \\ 0.603 & 0.230 & 0.167 \end{bmatrix} \quad (14)$$

$$t_n N_{4x4} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \end{bmatrix} = \left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} - \begin{bmatrix} x_0 \\ x_0 \\ x_0 \\ x_0 \end{bmatrix} \right) \qquad N_{4x4} = \begin{bmatrix} 0.278 & -0.202 & 0.169 & -0.071 \\ 0.398 & 0.069 & 0.064 & -0.031 \\ 0.387 & 0.234 & 0.278 & -0.071 \\ 0.389 & 0.222 & 0.389 & 0.000 \end{bmatrix}$$
(16) (17)

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \left(\tau \left(t_n N_{5x5} \right)^{-1} + I \right)^{-1} \tau \left(t_n N_{5x5} \right)^{-1} \begin{bmatrix} x_0 \\ x_0 \\ x_0 \\ x_0 \\ x_0 \\ x_0 \end{bmatrix} = \begin{bmatrix} 0.791 \\ 0.489 \\ 0.277 \\ 0.171 \\ 0.135 \end{bmatrix}$$
(22)

The explicit solution $x(t) = x_0 e^{-\frac{t}{\tau}}$ verifies that the numerical solution results are correct.

323 6. Conclusions

This tutorial paper serves as a guide to practitioners in relating the common 324 steps typically deployed in linear MPC applications to a comparable procedure 325 for nonlinear applications. The application in this paper is the quadruple tank 326 process that is a basic example of multivariate modeling and control. As a first 327 step, certain parameters of the model are adjusted to fit to PRBS data through 328 dynamic data reconciliation. In a next step, the controller is tuned to provide 329 desirable control responses for set point tracking and disturbance rejection. For 330 both estimation and control cases, alternate squared error and L_1 -norm error 331 forms are compared. While the L_1 -norm error uses additional variables and 332 equations, it adds only linear equality and inequality constraints. As a final 333 section of the tutorial, the process of converting differential equations into a set 334 of algebraic equations is reviewed. This conversion step is necessary to solve 335 the model and objective function simultaneously with NLP solvers. Along with 336 the tutorial overview, example MATLAB scripts are given in the Appendix as 337 a guide to implement the problems in the text. While this tutorial overview is 338 not an exhaustive review of all available techniques or software, it provides a 339 case study to advance the use of nonlinear models in control practice. 340

³⁴¹ Appendix A. Quadruple Tank Model

The quadruple tank process is represented by 14 differential and algebraic equations (DAEs). The following model is expressed in the APMonitor Modeling Language. This file and others included in the paper are available at APMonitor.com.

```
346
347
    Model
348
       Constants
         % gravitational constant (cm/s^2)
349
           = 981
350
           tank cross-sectional area (cm<sup>2</sup>)
351
                  = 28
         Area [1]
352
         Area 2
                  = 32
353
         Area [3]
                  = 28
354
         Area [4]
                  = 32
355
         % relation of level to voltage measurement (V/cm)
356
         kc = 0.50
357
      End Constants
358
```

```
359
360
          Parameters
             \% relation of input voltage to pump flow rate (cm^3/sec / V)
361
             km = 10.0, >=3.0, <=20.0 % slope
kb = 0.0, >=-20.0, <=20.0 % intercept
362
363
             kb = 0.0, >=-20.0, <=20.0 % intercept
% correction factors to fit model to real data
c13 = 0.071, >0.01, <=0.2 % outlet flow corrections
c24 = 0.057, >0.01, <=0.2 % outlet flow corrections
% fractional split to tank 1 vs. tank 4
364
365
366
367
              \begin{array}{l} & \text{gamma}[1] = 0.43, >=0, <=1 \\ & \text{fractional split to tank 2 vs. tank 3} \\ & \text{gamma}[2] = 0.34, >=0, <=1 \end{array} 
368
369
370
             % voltage to pump A
371
                                                       % Volt
372
              \texttt{v1} = 3\,, \ >=0, \ <=10
373
             \% voltage to pump B
                                                      % Volt
374
              v2 = 3, >=0, <=10
375
          End Parameters
376
377
           Variables
             \% tank height - diameter = 6 cm, max height = 20 cm
378
379
             {\tt h}\,[\,1\,] ~=~ 1\,2\,.\,6\,, ~>=1{\tt e}\,{-}5
380
             h[2] = 13.0, >=1e-5
             h[3] = 4.8 , >=1e-5
h[4] = 4.9 , >=1e-5
381
382
383
          End Variables
384
385
           Intermediates
             \% correction factors
386
387
              c[1] = c13
              c[2] = c24
388
             c[3] = c13 
 c[4] = c24
389
390
             % pump flows
391
              qa = v1 * km + kb
392
             qb = v2 * km + kb
% inlet flows from pumps
393
394
                   q[1] = gamma[1] * qa 
      q[2] = gamma[2] * qb 
      q[3] = (1-gamma[2]) * qb 
      q[4] = (1-gamma[1]) * qa 
      % outlet flows
395
396
397
398
399
              out [1:4] = c[1:4] * sqrt (2*g*h[1:4])
400
             % total inlet flows
401
             in [1] = q [1] + out [3] 
in [2] = q [2] + out [4] 
in [3] = q [3]
402
                                    + out [4]
403
404
              in[4] = q[4]
405
          End Intermediates
406
407
408
          Equations
              Area[1:4] * $h[1:4] = in[1:4] - out[1:4] % $ = differential
409
          End Equations
410
       End Model
411_{2}
```

⁴¹³ Appendix B. Parameter Estimation with a PRBS-Generated Signal

The following MATLAB script details the commands necessary to reproduce the parameter estimation case presented in this paper. The parameter estimation uses two elements including the model file (4tank.apm) and a data file (prbs360.csv). The model file is shown in Appendix A while the data file is available for download from APMonitor.com under the APM MATLAB examples section.

```
420
        % Add path to APM MATLAB libraries (available at APMonitor.com)
421
422
         addpath('../apm
% Clear MATLAB
                                      / apm ' ) ;
423
         clear all; close all;
% Server and Application name
424
425
          server = 'http://xps.apmonitor.com'; app = 'prbs';
426
          % Clear previous application
427
         apm(server,app, 'clear all');
% load model and data
428
429
         disp('Loading model'); apm_load(server,app, '4tank.apm');
disp('Loading data'); csv_load(server,app, 'prbs360.csv');
% Set up variable classifications for data flow
% Feedforwards - measured process disturbances
430
431
432
433
        % Feedforwards - measured process dist
apm_info(server, app, 'FV', 'km');
apm_info(server, app, 'FV', 'kb');
apm_info(server, app, 'FV', 'gamma[1]');
apm_info(server, app, 'FV', 'c13');
apm_info(server, app, 'FV', 'c24');
% State variables (for display only)
apm_info(server, app, 'SV', 'h[3]');
apm_info(server, app, 'SV', 'h[3]');
apm_info(server, app, 'SV', 'h[4]');% Controlled variables (for controlled
434
435
436
437
438
439
440
441
442
         % Controlled variables (for controller design)
apm_info(server,app, 'CV', 'h[1]');
apm_info(server,app, 'CV', 'h[2]');
443
444
445
446
          % imode (1=ss, 2=mpu, 3=rto, 4=sim, 5=est, 6=ctl)
447
          apm_option(server, app, 'nlc.imode', 5);
448
          % read csv file
449
          apm_option(server, app, 'nlc.csv_read',1);
         % estimated variable error type (1=L1-norm, 2=Squared Error)
450
         apm_option(server,app,'nlc.ev_type',2);

% time units (1=sec, 2=min, 3=hrs, 4=days, etc)

apm_option(server,app,'nlc.ctrl_units',1);

apm_option(server,app,'nlc.hist_units',2);
451
452
453
454
           % parameters to adjust
455
          apm_option(server, app, 'km.status ',1);
apm_option(server, app, 'km.lower',3);
apm_option(server, app, 'km.upper',20);
apm_option(server, app, 'kb.status ',1);
456
457
458
459
         apm_option(server, app, 'kb.status ',1);
apm_option(server, app, 'kb.upper', 2);
apm_option(server, app, 'gamma[1].status',1);
460
461
        apm_option(server, app, 'gamma[1].status',1);
apm_option(server, app, 'gamma[1].lower',0.2);
apm_option(server, app, 'gamma[1].lower',0.8);
apm_option(server, app, 'gamma[2].status',1);
apm_option(server, app, 'gamma[2].lower',0.2);
apm_option(server, app, 'c13.status',1);
apm_option(server, app, 'c13.lower',0.01);
apm_option(server, app, 'c13.lower',0.01);
apm_option(server, app, 'c13.lower',0.2);
apm_option(server, app, 'c24.status',1);
apm_option(server, app, 'c24.status',1);
apm_option(server, app, 'c24.lower',0.01);
apm_option(server, app, 'c24.lower',0.2);
% measured values for model fitting
apm_option(server, app, 'h[1].fstatus',1);
462
463
464
465
466
467
468
469
470
471
472
473
474
         apm_option(server,app, 'h[1].fstatus',1);
apm_option(server,app, 'h[2].fstatus',1);
% solver (1=APOPT, 3=IPOPT)
475
476
477
478
          \verb"apm_option(server, app, 'nlc.solver', 3);
         % Solve with APMonitor
479
480
          apm(server, app, 'solve')
481
          % Open web-viewer
482
          apm_web(server, app);
         \% Retrieve solution (creates solution.csv locally)
483
484
          solution = apm_sol(server, app);
```

486 Appendix C. Nonlinear Control of the Quadruple Tank Process

The following MATLAB script details the commands necessary to reproduce
the nonlinear controller presented in this paper. The model file is the same as
is shown in Appendix A but updated with updated parameters from Table 3.
The APM MATLAB libraries are available for download from APMonitor.com.

```
491
492
         % Add path to APM libraries
         addpath('../apr
% Clear MATLAB
493
                                   / apm ' );
494
495
         clear all; close all;
         % Server and Application Name
496
         server = 'http://xps.apmonitor.com'; app = 'nlc';
% Clear previous application
497
498
         apm(server,app,'clear all');
% load model with updated parameters
499
500
         apm_load(server, app, '4tank.apm');
% load future time horizon
501
502
         % Set up variable classifications for data flow
503
504
        % Feedforwards - measured process parameters
apm_info(server,app,'FV','gamma[1]');
apm_info(server,app,'FV','gamma[2]');
% Manipulated variables (for controller design)
505
506
507
508
         apm_info(server, app, 'MV', 'v1');
apm_info(server, app, 'MV', 'v2');
% State variables (for display only)
apm_info(server, app, 'SV', 'h[3]');
apm_info(server, app, 'SV', 'h[4]');
509
510
511
512
513
         % Controlled variables (for controller design)
apm_info(server,app, 'CV', 'h[1]');
apm_info(server,app, 'CV', 'h[2]');
514
515
516
        % steady state initialization
% imode = 3, steady state mode
517
518
        apm_option(server,app,'nlc.imode',3);
apm(server,app,'solve');
% imode = 6, switch to dynamic control
apm_option(server,app,'nlc.imode',6);
% nodes = 3, internal nodes in the collocation structure (2-6)
519
520
521
522
523
524
         \verb"apm_option(server, app, 'nlc.nodes', 3);
         % time units (1=sec, 2=min, etc)
525
         apm_option(server,app, 'nlc.ctrl_units',1); % controller time units
apm_option(server,app, 'nlc.hist_units',2); % units for trending
% read csv file
526
527
528
         apm_option(server, app, 'nlc.csv_read', 1);
529
            Manipulated variable tuning
530
         apm_option(server, app, 'v1. status ',1); % turn on v1
apm_option(server, app, 'v1. upper ',6); % upper bound
apm_option(server, app, 'v1. lower ',1); % lower bound
apm_option(server, app, 'v1. dmax',1); % max move pe
apm_option(server, app, 'v1. dcost ',1); % movement pe
apm_option(server, app, 'v2. status ',1); % turn on v2
531
532
533
534
                                                                                                    % max move per cycle
535
                                                                                                  % movement penalty
536
         apm_option(server,app, 'v2.status ,1); % turn on v2
apm_option(server,app, 'v2.upper',6); % upper bound
apm_option(server,app, 'v2.lower',1); % lower bound
apm_option(server,app, 'v2.dmax',1); % max move per cyc
apm_option(server,app, 'v2.dcost',1); % movement penalty
537
538
                                                                                                    % max move per cycle
539
540
         % Controlled variable tuning
541
         apm_option(server,app, 'h[1].status',1); % turn on h[1]
apm_option(server,app, 'h[1].fstatus',0); % turn off feedback status
542
543
         apm_option(server, app, 'h[1]. istatus ,0); % turn on needback status
apm_option(server, app, 'h[1]. isphi', 10.1); % setpoint high
apm_option(server, app, 'h[1]. splo', 9.9); % setpoint low
apm_option(server, app, 'h[1]. tau', 10); % speed of response
apm_option(server, app, 'h[2]. status', 1); % turn on h[2]
apm_option(server, app, 'h[2]. fstatus', 0); % turn on h[2]
544
545
546
547
548
         apm_option(server, app, 'h[2].sphi', 15.1); % setpoint high
549
```

```
apm_option(server, app, 'h[2].splo', 14.9); \% setpoint low
550
    apm_option(server, app, 'h[2].tau', 10);
                                                 % speed of response
551
    % Set controller mode
552
    apm_option(server, app, 'nlc.reqctrlmode',3);
553
554
    6 Run APMonitor
    apm(server, app, 'solve')
555
556
    % Open web-viewer
557
    apm_web(server, app);
      Retrieve solution (creates solution.csv locally)
558
    solution = apm_sol(server, app);
558
```

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