

## PROCCEDINGS

| 10 - 13 September 2007

# FACULTY OF COMPUTER SCIENCE AND AUTOMATION



# **COMPUTER SCIENCE MEETS AUTOMATION**

# **VOLUME I**

- **Session 1 Systems Engineering and Intelligent Systems**
- Session 2 Advances in Control Theory and Control Engineering
- Session 3 Optimisation and Management of Complex Systems and Networked Systems
- **Session 4 Intelligent Vehicles and Mobile Systems**
- **Session 5 Robotics and Motion Systems**



## Bibliografische Information der Deutschen Bibliothek

Die Deutsche Bibliothek verzeichnet diese Publikation in der deutschen Nationalbiografie; detaillierte bibliografische Daten sind im Internet über http://dnb.ddb.de abrufbar.

#### ISBN 978-3-939473-17-6

#### Impressum

Herausgeber:	Der Rektor der Technischen Universität Ilmenau UnivProf. Dr. rer. nat. habil. Peter Scharff
Redaktion:	Referat Marketing und Studentische Angelegenheiten Kongressorganisation Andrea Schneider Tel.: +49 3677 69-2520 Fax: +49 3677 69-1743 e-mail: kongressorganisation@tu-ilmenau.de
Redaktionsschluss:	Juli 2007
Verlag:	Co Technische Universität Ilmenau/Universitätsbibliothek Universitätsverlag Ilmenau Postfach 10 05 65 98684 Ilmenau www.tu-ilmenau.de/universitaetsverlag
Herstellung und Auslieferung:	Verlagshaus Monsenstein und Vannerdat OHG Am Hawerkamp 31 48155 Münster www.mv-verlag.de
Layout Cover:	www.cey-x.de
Bezugsmöglichkeiten:	Universitätsbibliothek der TU Ilmenau Tel.: +49 3677 69-4615 Fax: +49 3677 69-4602

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#### Preface

Dear Participants,

Confronted with the ever-increasing complexity of technical processes and the growing demands on their efficiency, security and flexibility, the scientific world needs to establish new methods of engineering design and new methods of systems operation. The factors likely to affect the design of the smart systems of the future will doubtless include the following:

- As computational costs decrease, it will be possible to apply more complex algorithms, even in real time. These algorithms will take into account system nonlinearities or provide online optimisation of the system's performance.
- New fields of application will be addressed. Interest is now being expressed, beyond that in "classical" technical systems and processes, in environmental systems or medical and bioengineering applications.
- The boundaries between software and hardware design are being eroded. New design methods will include co-design of software and hardware and even of sensor and actuator components.
- Automation will not only replace human operators but will assist, support and supervise humans so that their work is safe and even more effective.
- Networked systems or swarms will be crucial, requiring improvement of the communication within them and study of how their behaviour can be made globally consistent.
- The issues of security and safety, not only during the operation of systems but also in the course of their design, will continue to increase in importance.

The title "Computer Science meets Automation", borne by the 52<sup>nd</sup> International Scientific Colloquium (IWK) at the Technische Universität Ilmenau, Germany, expresses the desire of scientists and engineers to rise to these challenges, cooperating closely on innovative methods in the two disciplines of computer science and automation.

The IWK has a long tradition going back as far as 1953. In the years before 1989, a major function of the colloquium was to bring together scientists from both sides of the Iron Curtain. Naturally, bonds were also deepened between the countries from the East. Today, the objective of the colloquium is still to bring researchers together. They come from the eastern and western member states of the European Union, and, indeed, from all over the world. All who wish to share their ideas on the points where "Computer Science meets Automation" are addressed by this colloquium at the Technische Universität Ilmenau.

All the University's Faculties have joined forces to ensure that nothing is left out. Control engineering, information science, cybernetics, communication technology and systems engineering – for all of these and their applications (ranging from biological systems to heavy engineering), the issues are being covered.

Together with all the organizers I should like to thank you for your contributions to the conference, ensuring, as they do, a most interesting colloquium programme of an interdisciplinary nature.

I am looking forward to an inspiring colloquium. It promises to be a fine platform for you to present your research, to address new concepts and to meet colleagues in Ilmenau.

In Sherte

Professor Peter Scharff Rector, TU Ilmenau

"L. Ummt

Professor Christoph Ament Head of Organisation

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H. Gerbracht/ P. Li/ W. Hong

# An efficient optimization approach to optimal control of large-scale processes

## INTRODUCTION

In this contribution, we consider the interior-point quasi-sequential approach as an efficient optimization method to handle optimal control problems of large-scale processes. This approach is an extension of the quasi-sequential approach [1]. In the original quasi-sequential approach an active-set strategy was applied. In this work an interior-point strategy for the efficient solution of large-scale dynamic optimization problems will be proposed. Numerical experiments showed that with an increasing number of active constraints the computational effort rises significantly (for detailed results see [1]). This high computational costs are a result of the active-set implemented in the recent quasi–sequential approach. Typically the finding of an active-set represents a massive combinatorial problem if the number of active constraints is high [3]. Therefore for this type of processes the active-set line-search strategy is not suitable. An alternative line-search strategy, the interior-point method, does not result in a comparable increase in computational cost in similar circumstances.

## STATE-OF-THE-ART

Dynamic optimization approaches can be divided in two main branches, the direct and indirect methods. Current research concentrates on the direct methods. They can be distinguished in simultaneous, sequential and combined approaches. The combined approaches integrate the advantages of both, simultaneous and sequential, methods. Two well known combinations of those approaches exist: the multiple-shooting approach [4] and the quasi-sequential approach [1].

The fundamental advantages of the quasi-sequential approach are the following: On the one hand it is possible to maintain the path constraints of state variables. In the simultaneous approach the maintaining of this path constraints is realized by including

the state and control variables on discrete time points in the optimization. In the quasisequential approach, however, this is ensured by enforcing the equality and inequality constraints at the collocation points in the NLP solver. On the other hand only a smallscale NLP solver is needed as in sequential approaches and in terms of real-time optimization it is important that a feasible path strategy is used is used in the quasisequential framework.

#### **QUASI-SEQUENTIAL INTERIOR-POINT METHOD**

The quasi-sequential approach is divided in two layers, the simulation and optimization layer. In the simulation layer both control and state variables are discretized by orthogonal collocation, the equality constraints are solved by a Newton solver and the sensitivities and gradients are calculated. The elimination of the equality constraints by simulation simplifies the line-search problem in the optimization layer considerably and therefore larger steps can be taken towards the optimum. Only the control variables and inequalities are included in the optimization layer. Hence, if we want to modify the line-search method, which is a part of the optimization algorithm, the simulation layer can stay unchanged.

Until now the SQP based IMSL<sup>®</sup> routine DNCONG, which includes an active-set linesearch strategy, has been used as the small-scale NLP solver in the optimization layer. This routine has to be replaced for the implementation of the interior-point method. In place of the DNCONG a primal-dual interior-point method (adapted from [2]) with a generalized augmented Lagrangian function as a merit function, which shows excellent convergence properties and computational performances, is employed. Due to the handling of inequality constraints with barrier terms the problem to be solved consists merely of an objective function. This leads to a considerable reduction of computational costs in situations where the number of active constraints is high. In the following section the developed algorithm will be explained in detail.

We consider a general NLP problem by approximating state profiles with orthogonal collocation on finite elements (time intervals) of the form

$$\min_{u \in \mathbb{R}^{n-m}} f(z(u_{l,i}), u_{l,i})$$
s.t.
$$g_{l,i} (z(u_{l,i}), u_{l,i}) = 0$$

$$u_L \le u_{l,i} \le u_U$$

$$z_L \le z(u_{l,i}) \le z_U$$
(1)

where i = 1, ..., NC and l = 1, ..., NL are the encounter for the collocation points and the time intervalls of the discretization, respectively.  $u \in \mathbb{R}^{n-m}$  and  $z(u) \in \mathbb{R}^m$  are the control (independent) and state (dependent) variables,  $f(z(u_{l,i}), u_{l,i}) : \mathbb{R}^n \to \mathbb{R}$  is the objective function and  $g(z(u_{l,i}), u_{l,i}) : \mathbb{R}^n \to \mathbb{R}^m$  are the equality constraints.  $u_L, z_L$  and  $u_U, z_U$  are the lower and upper bounds of the control and state variables.

The equality constraints will be solved through simulation of the model equations, which provides the state variables  $z(u_{l,i})$  for each collocation point. Additionally the inequality constraints will be replaced by logarithmic barrier terms that have been added to the objective function. The resulting optimization problem is

$$\min_{u \in \mathbb{R}^{n-m}} \varphi_{\mu} \left( z(u_{l,i}), u_{l,i} \right) = f \left( z(u_{l,i}), u_{l,i} \right) - \mu \left\{ \sum_{j=1}^{n-m} \ln \left[ u_{l,i}^{(j)} - u_L \right] + \sum_{j=1}^{n-m} \ln \left[ u_U - u_{l,i}^{(j)} \right] + \sum_{j=1}^{m} \ln \left[ z(u_{l,i})^{(j)} - z_L \right] + \sum_{j=1}^{m} \ln \left[ z_U - z(u_{l,i})^{(j)} \right] \right\}$$
(2)

with the barrier parameter  $\mu > 0$  as well as  $u_{l,i}^{(j)}$  and  $z(u_{l,i})^{(j)}$  as the *j*th component of the vector  $u_{l,i}$  and  $z(u_{l,i})$ . If we modify notation with  $u_{l,i} = u$  and  $z(u_{l,i}) = z(u)$  as the vectors of all discretized control and state variables, the following Lagrange function can be defined:

$$\mathcal{L}\left(z(u), u, \nu^{L}, \nu^{U}\right) = f(z(u), u) - \sum_{j=1}^{n-m} \nu^{LU} \left[u^{(j)} - u_{L}\right] - \sum_{j=1}^{n-m} \nu^{UU} \left[u_{U} - u^{(j)}\right] - \sum_{j=1}^{m} \nu^{LZ} \left[z(u)^{(j)} - z(u)_{L}\right] - \sum_{j=1}^{m} \nu^{UZ} \left[z(u)^{(j)} - z(u)_{L}\right], \quad (3)$$

where  $(\nu^L)^T = \left[ (\nu^{LZ})^T (\nu^{LU})^T \right]$  and  $(\nu^U)^T = \left[ (\nu^{UZ})^T (\nu^{UU})^T \right]$  are the Lagrange multipliers for the lower and upper bounds of the state and control variables as stated in (1). The related optimality conditions can be written as follows

$$\nabla_{u} f(z(u), u) - \nu^{LU} + \nu^{UU} - (\nu^{LZ})^{T} \frac{dz(u)}{du} + (\nu^{UZ})^{T} \frac{dz(u)}{du} = 0$$
  
$$\nabla_{z} f(z(u), u) - \nu^{LZ} + \nu^{UZ} = 0$$
  
$$[U - U_{L}] V^{LU} e - \mu e = 0$$
  
$$[U_{U} - U] V^{UU} e - \mu e = 0$$
  
$$[Z - Z_{L}] V^{LZ} e - \mu e = 0$$
  
$$[Z_{U} - Z] V^{UZ} e - \mu e = 0$$

with  $[U - U_L]$ ,  $[U_U - U]$ ,  $[Z - Z_L]$ ,  $[Z_U - Z]$  and V as diagonal matrices with the related entries on their diagonals and  $e = [1, ..., 1]^T$  in the adequate dimension. The optimality conditions are solved with a Newton method. The search directions  $(d_k^z, d_k^u, d_k^{LU}, d_k^{UU}, d_k^{LZ}, d_k^{UZ})$  at an iteration  $(z(u)_k, u_k, \nu_k^{LU}, \nu_k^{UU}, \nu_k^{LZ}, \nu_k^{UZ})$  are obtained by linearization of the optimality conditions:

$$\begin{bmatrix} W_{UZ,k} & W_{UU,k} & -I & I & -\left(\frac{dz}{du}\right)_{k}^{T} & \left(\frac{dz}{du}\right)_{k}^{T} \\ W_{ZZ,k} & W_{ZU,k} & 0 & 0 & -I & I \\ 0 & V_{k}^{LU} & [U - U_{L}]_{k} & 0 & 0 & 0 \\ 0 & -V_{k}^{UU} & 0 & [U_{U} - U]_{k} & 0 & 0 \\ V_{k}^{LZ} & 0 & 0 & 0 & [Z - Z_{L}]_{k} & 0 \\ -V_{k}^{UZ} & 0 & 0 & 0 & 0 & [Z_{U} - Z]_{k} \end{bmatrix} \begin{bmatrix} d_{k}^{z} \\ d_{k}^{U} \\ d_{k}^{UU} \\ d_{k}^{UZ} \\ d_{k}^{UZ} \end{bmatrix}$$
$$= -\begin{bmatrix} \nabla_{u}f(z(u_{k}), u_{k}) - \nu_{k}^{LU} + \nu_{k}^{UU} - \left(\nu_{k}^{LZ}\right)^{T} \frac{dz(u)}{du} + \left(\nu_{k}^{UZ}\right)^{T} \frac{dz(u)}{du} \\ \nabla_{u}f(z(u_{k}), u_{k}) - \nu_{k}^{LU} + \nu_{k}^{UU} - \left(\nu_{k}^{LZ}\right)^{T} \frac{dz(u)}{du} + \left(\nu_{k}^{UZ}\right)^{T} \frac{dz(u)}{du} \\ \end{bmatrix} \begin{bmatrix} (4) \\ [U - U_{L}]_{k} V_{k}^{LU} e - \mu e \\ [U_{U} - U]_{k} V_{k}^{LU} e - \mu e \\ [Z_{U} - Z_{L}]_{k} V_{k}^{LZ} e - \mu e \end{bmatrix} \end{bmatrix}$$

where  $W_k = \nabla^2 \mathcal{L} \left( z(u)_k, u_k, \nu_k^{LU}, \nu_k^{UU}, \nu_k^{LZ}, \nu_k^{UZ} \right)$  is the Hessian of the Lagrange function with respect to the mentioned indices. Eliminating  $\nu_k^{LU}, \nu_k^{UU}, \nu_k^{LZ}$  and  $\nu_k^{UZ}$  leads to the following system

$$\begin{bmatrix} W_{UZ,k} + \Sigma_{UZ,k} & W_{UU,k} + \Sigma_{UU,k} \\ W_{ZZ,k} + \Sigma_{ZZ,k} & W_{ZU,k} + \Sigma_{ZU,k} \end{bmatrix} \begin{bmatrix} d_k^z \\ d_k^u \end{bmatrix} = -\begin{bmatrix} \nabla_u \varphi_\mu(z(u_k), u_k) \\ \nabla_z \varphi_\mu(z(u_k), u_k) \end{bmatrix}$$
(5)

with

$$\Sigma_{UZ,k} = [Z - Z_L]_k^{-1} \left(\frac{dz}{du}\right)_k^T V_k^{LZ} + [Z_U - Z]_k^{-1} \left(\frac{dz}{du}\right)_k^T V_k^{UZ}$$
  

$$\Sigma_{UU,k} = [U - U_L]_k^{-1} V_k^{LU} + [U_U - U]_k^{-1} V_k^{UU}$$
  

$$\Sigma_{ZZ,k} = [Z - Z_L]_k^{-1} V_k^{LZ} + [Z_U - Z]_k^{-1} V_k^{UZ}$$
  

$$\Sigma_{ZU,k} = 0$$

and

$$\begin{aligned} d_k^{LU} &= -V_k^{LU}e + [U - U_L]^{-1} \left(\mu e - V_k^{LU} d_k^u\right) \\ d_k^{UU} &= -V_k^{UU}e + [U_U - U]^{-1} \left(\mu e + V_k^{UU} d_k^u\right) \\ d_k^{LZ} &= -V_k^{LZ}e + [Z - Z_L]^{-1} \left(\mu e - V_k^{LZ} d_k^z\right) \\ d_k^{UZ} &= -V_k^{UZ}e + [Z_U - Z]^{-1} \left(\mu e + V_k^{UZ} d_k^z\right) \end{aligned}$$

as the search directions for the Lagrange multipliers. Additionally in comparison to [2] in  $\Sigma_k$  the sensitivities have been considered.  $d_k^z$  and  $d_k^u$  can be obtained by the solution of the following QP subproblem:

$$\min_{d \in \mathbb{R}^n} \nabla \varphi\left(x_k\right) d_k^x + \frac{1}{2} \left(d_k^x\right)^T \left(W_k + \Sigma_k\right) d_k^x \tag{6}$$

with  $x^T = (z^T u^T)$  for better readability. Note that, in contrast to [2], this optimization problem contains no equality constraints. The solution can directly be calculated as

$$d_k^x = -(W_k + \Sigma_k)^{-1} \nabla \varphi(x_k)$$
(7)

In order to obtain the next iterate the step sizes  $\alpha_k \in (0, \alpha_k^{max}], \alpha_k^{\nu} \in (0, 1]$  must be determined. A first approximation for the step-length is given by the *fraction-to-the-boundary* rule to maintain the positivity of the variables:

$$\begin{aligned}
\alpha_{k}^{max} &:= \max \left\{ \alpha \in (0,1] : z(u_{k}) + \alpha d_{k}^{z} \ge (1-\tau_{j}) z(u_{k}) \right\} \\
\alpha_{k}^{max} &:= \max \left\{ \alpha \in (0,1] : u_{k} + \alpha d_{k}^{u} \ge (1-\tau_{j}) u_{k} \right\} \\
\alpha_{k}^{\nu} &:= \max \left\{ \alpha \in (0,1] : \nu_{k}^{L} + \alpha d_{k}^{\nu_{L}} \ge (1-\tau_{j}) \nu_{k}^{L} \right\} \\
\alpha_{k}^{\nu} &:= \max \left\{ \alpha \in (0,1] : \nu_{k}^{U} + \alpha d_{k}^{\nu_{U}} \ge (1-\tau_{j}) \nu_{k}^{U} \right\}
\end{aligned}$$
(8)

where  $\tau_j = max \{\tau_{min}, 1 - \mu_j\} \in (0, 1)$  is the *fraction-to-the-boundary* parameter [2]. A sufficient decrease condition on a merit function is used to give an second approximation for the step-length by applying the *Armijo condition*:

 $M_{\mu_k}\left(x_{k+1}, \nu_{k+1}^L, \nu_{k+1}^U; \rho\right) \leq M_{\mu_k}\left(x_k, \nu_k^L, \nu_k^U; \rho\right) + c_k \alpha_k \beta \nabla \Phi_{\mu_k}\left(x_k, \nu_k^L, \nu_k^U; \rho\right) \Delta x_k \quad (9)$ with  $x^T = (z^T u^T), \nu_L^T = (\nu_{LZ}^T \nu_{LU}^T), \nu_U^T = (\nu_{UZ}^T \nu_{UU}^T), c > 0, \ \beta \in (0, 1) \text{ and } \alpha_k = p^t \alpha_k^{max}$ , where t is the smallest nonnegative integer value such that  $\alpha_k$  satisfies the above condition [5]. For any  $\mu > 0$  the merit function  $M_{\mu}$  is defined by

$$M_{\mu}(x,\nu_{l},\nu_{U};\rho) = \mathcal{L}(x,\nu_{L},\nu_{U}) + \rho \Phi_{\mu}(x,\nu_{L},\nu_{U})$$
(10)

where  $\rho$  is a nonnegative penalty parameter and  $\Phi_{\mu}$  is the penalty term

$$\Phi_{\mu}(x,\nu_{L},\nu_{U}) = \nu_{L}^{T}[x-x_{L}] + \nu_{U}^{T}[x_{U}-x] -\mu \left\{ \sum_{j=1}^{n} \ln\left(\nu_{L,j}[x-x_{L}]_{j}\right) + \sum_{j=1}^{n}\left(\nu_{U,j}[x_{U}-x]_{j}\right) \right\}$$
(11)

In Eq. (10) the penalty parameter  $\rho = \tilde{\rho} + c$  is calculated by

$$\tilde{\rho} = \frac{\nabla_x \mathcal{L}^T \Delta x + \nabla_{\nu_L} \mathcal{L}^T \Delta \nu_L + \nabla_{\nu_U} \mathcal{L}^T \Delta \nu_U}{\nabla \Phi_\mu^T \Delta x}$$
(12)

with a given *c*. In the global line-search interior-point algorithm with given  $\tilde{c} > 0$  and  $\rho$  the current penalty parameter to update  $\rho$  is

$$\rho_{+} = \begin{cases} \tilde{\rho}_{+} + \tilde{c}, & \text{if } \tilde{\rho}_{+} + \tilde{c} > \rho, \\ \tilde{\rho}_{+} + c, & \text{otherwise,} \end{cases}$$
(13)

where  $\tilde{\rho}_+$  is given by (12),  $c = \rho - \tilde{\rho}_+$  and  $c \ge \tilde{c}$ . After calculating the search direction the variables for the next iterate will be determined and the damped BFGS update for the matrix  $W_k + \Sigma_k$  is taken from [6]. After that it will be checked if  $(x_k, \nu_{L,k}, \nu_{U,k}) \notin \mathcal{N}_{\mu_k}(\gamma)$ . If this condition is satisfied, then repeat the inner loop by going back to Eq. (6).  $\mathcal{N}_{\mu_k}(\gamma)$  is defined as a neighborhood of a point of the quasicentral path [5] corresponding to  $\mu$  by

$$\mathcal{N}_{\mu}(\gamma) = \left\{ (x, \nu_L, \nu_U) \in \mathbb{R}^{3n} : x > 0, \ \nu_L > 0, \ \nu_U > 0, \\ \left\| w_L - \mu w_L^{-1} \right\|^2 + \left\| w_U - \mu w_U^{-1} \right\|^2 \le \gamma \mu \right\}$$
(14)

with  $w_L = \{ [X - X_L] V^L e \}^{\frac{1}{2}}, w_U = \{ [X_U - X] V^U e \}^{\frac{1}{2}} \text{ and } (\mu, \gamma) > 0. \text{ Otherwise } \mu \text{ is } \}$ updated on the following way:

$$\mu_{k+1} = \sigma \left( \left\| w_{L,k} - \mu_k w_{L,k}^{-1} \right\|^2 + \left\| w_{U,k} - \mu_k w_{U,k}^{-1} \right\|^2 \right),$$
(15)

where  $\sigma \in (0,1)$  is choosen by the user. This loop will be repeated until the following stopping criteria is satisfied:

$$\epsilon_{tol} \geq max \quad \left\{ \left\| \nabla_{u} f(z(u), u) - \nu^{LU} + \nu^{UU} - (\nu^{LZ})^{T} \frac{dz}{du} + (\nu^{UZ})^{T} \frac{dz}{du} \right\|_{\infty}, \\ \left\| \nabla_{z} f(z(u), u) - \nu^{LZ} + \nu^{UZ} \right\|_{\infty}, \\ \left\| [X - X_{L}] V^{L} e - \mu e \right\|_{\infty}, \\ \left\| [X_{U} - X] V^{U} e - \mu e \right\|_{\infty} \right\}$$
(16)

with  $\epsilon_{tol} > 0$  as a user provided error tolerance. Additionally, if there arise numerical problems, it is possible to modify the stopping criteria by scaling factors [2]. The proposed approach has been applied to the dynamic optimization of a continuous stirred-tank reactor (CSTR) and a heat-integrated distillation column system [1].

#### CONCLUSION

In this work an efficient interior-point method for large-scale optimization problems has been proposed. This approach has been implemented in the guasi-sequential framework in order to substitute the recent active-set strategy, which has a low performance for large-scale problems with many active inequality constraints. Further research could be done by comparing some of those methods or modify them, e.g. introducing slack variables, to reach an additional decrease in computational costs. Another area of research could be the application of the quasi-sequential approach to instable processes.

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