OPTCON: AN ALGORITHM FOR SOLVING UNCONSTRAINED CONTROL PROBLEMS

By

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To my wonderful parents Zhanwu Li and Peirong Zheng.

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Abstract of Thesis Presented to the Graduate School
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OPTCON: AN ALGORITHM FOR SOLVING UNCONSTRAINED CONTROL PROBLEMS

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Recently, Dr. Hager and Hongchao Zhang developed a new optimization algorithm-CG_DESCENT. In this project, we show how CG_DESCENT can be used to solve unconstrained optimal control problems. The resulting algorithm is called OPTCON.

This numerical work is meaningful, since optimal control applications appear in so many fields, such as aerospace, electronic circuits, heat conduction, energy optimization and so on. These problems are usually complicated, with a large number of variables, parameters and initial values. Therefore, without a good numerical method, we barely can solve them by hand. This urges us to search for a fast yet stable method with less memory requirement and high accuracy.

Comparisons with another conjugate gradient method will be provided.

CHAPTER 1
INTRODUCTION

Based on the recent research of Dr. William W. Hager and Hongchao Zhang, a new conjugate gradient method CG_DESCENT was produced. (See the related paper [1].) This method can obtain even higher convergence speed than the ordinary conjugate gradient method and has relatively low memory requirement during the computation. In this master's thesis, we will employ the new conjugate gradient method to obtain a new method-OPTCON for solving nonlinear optimal control problems.

1.1 Terminology

We first define several terms that are used throughout this thesis. Consider an unconstrained optimal control problem of the form:

(1.0.1) minimize $J = \phi(x(t_f))$

(1.0.2) subject to: $\dot{x}(t) = f(x(t),u(t),t)$, $t \in [t_0, t_f]$

(1.0.3) $x(t_0) = \boldsymbol{\alpha}$,

where $x(t) \in \mathbf{R}^{nx}$, $\dot{x}(t)$ means $\frac{d}{dt}x$, and $u(t) \in \mathbf{R}^{nc}$, $f : \mathbf{R}^{nx} \times \mathbf{R}^{nc} \to \mathbf{R}^{nx}$, and $\phi : \mathbf{R}^{nx} \to \mathbf{R}$.

J is a function that evaluates the system performance or *system cost*. (1.0.2) is called the *system dynamics*, which is a group of differential equations for $x(t) \in \mathbf{R}^{nx}$, the *state variable*. The variable $u(t)$ is the *control variable*, which is used to optimize the *system cost*. The system has an *initial time* t_0, and a *final time* t_f. Our numerical work

only focuses on problems for which the *initial condition* (1.0.3) is given. Note that some problems have a *final condition* ($x(t_f) = x_f$).

1.2 Overview

The organization of the thesis is as follows:

In Chapter 2, we will first provide a study of the numerical technique that we used to solve the optimal control problem. Then, we will discover why CG_DESCENT method is a good option for the optimization. In Chapter 3, I will introduce a C program called OPTCON, which is the software developed for solving the practical problems with the new method. Comparison will be made for the performance of this new method relative to other conjugate gradient method. In Chapter 4, we will do some numerical experiments with the new method by perturbing the parameters in OPTCON to obtain the best performance for the sample problems.

CHAPTER 2
OPTIMAL CONTROL PROBLEMS

2.1 Discrete-time Systems And Runge-Kutta Discretization

In [2], a Runge-Kutta discretization and its convergence were analized for unconstrained control problems. To discretize the unconstrained optimal control problem (1.0.1)-(1.0.3), we use the uniform mesh of time interval, which has the length $h = \frac{t_f - t_0}{N}$, $N \in \mathbf{N}$. Now, if we apply an $s-stage$ Runge-Kutta integration scheme [3] with coefficients a_{ij} and b_i, $1 \le i, j \le s$ to the system dynamics (1.0.2), it becomes:

(2.1.1) $$x_k' = \sum_{i=1}^{s} b_i f(y_i, u_{ki}),$$

where $$x_k' = \frac{x_{k+1} - x_k}{h},$$

(2.1.2) $$y_i = x_k + h\sum_{j=1}^{s} a_{ij} f(y_j, u_{kj}),\ 1 \le i \le s,\ 0 \le k \le N-1.$$

Therefore, the discrete control problem is the following:

(2.1.3) minimize $J = \phi(x_N)$

(2.1.4) subject to $x_k' = \sum_{i=1}^{s} b_i f(y_i, u_{ki})$, where $x_0 = \boldsymbol{\alpha}$,

$$y_i = x_k + h\sum_{j=1}^{s} a_{ij} f(y_j, u_{kj}),\ 1 \le i \le s,\ 0 \le k \le N-1.$$

Since $x_k' = \frac{x_{k+1} - x_k}{h}$, x_N in (2.1.3) is obtained by solving the *state equation*:

(2.1.5) $$x_{k+1} = x_k + h\sum_{i=1}^{s} b_i f(y_i, u_{ki}), \text{ where } y_i = x_k + h\sum_{j=1}^{s} a_{ij} f(y_j, u_{kj}),$$

$$1 \le i \le s,\ 0 \le k \le N-1, \text{ and } x_0 = \boldsymbol{\alpha}.$$

Now, we explain how to compute the gradient of the cost function $\phi(x_N)$ with respect to the discrete control. To start we introduce the associated *costate equation*:

(2.1.6) $$\psi_k = \psi_{k+1} + h\sum_{i=1}^{s} b_i \chi_i \nabla_x f(y_i, u_{ki}),\ \ \psi_N = \nabla_x \phi(x_N)$$

(2.1.7) $$\text{where } \chi_i = \psi_{k+1} + \sum_{j=1}^{s} \frac{a_{ji}}{b_i} \lambda_j,$$

(2.1.8) $$\lambda_j = h b_j \chi_j \nabla_x f(y_j, u_{kj}).$$

As shown in [2],

(2.1.9) $$\nabla_{u_{kj}} \phi(u) = h b_j \chi_j \nabla_u f(y_j, u_{kj}).$$

Above formulas are employed in our OPTCON to evaluate the function cost and function gradient. For our numerical work, we assume the Runge-Kutta scheme is explicit. The conditions for the explicit 2nd, 3rd, and 4th order of a Runge-Kutta discretization can be found in [2] (Table 1).

2.2 Numerical Solution Methods

Analytic solution or accurate solution of optimal control problem is hard to obtain due to the complexity of the cost function $J(u)$ and the system dynamics $f(x(t), u(t), t)$. In most practical problems, numerical optimization method must be used. Basically, the flow chart for solving the optimal control problem is the following:

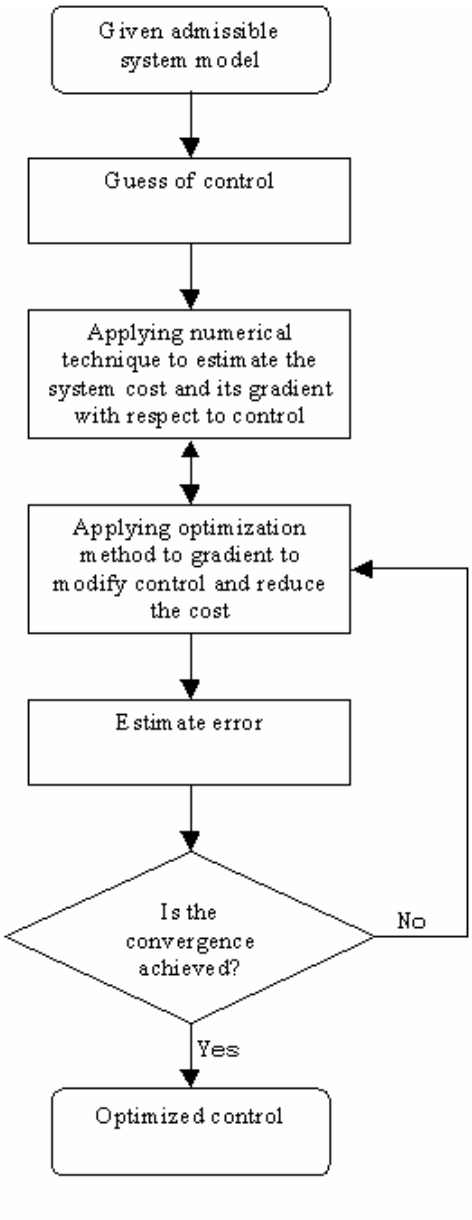

Figure 2-1. Flow chart of solving optimal control problems

There are many methods can be applied in the optimization process. Gradient or steepest descent method is one of the oldest and most obvious methods, but experience has shown that this method can be extremely slow. Conjugate gradient method such as feasible direction method and gradient projection method can be applied to our project. We will compare gradient projection method with Dr. Hager and Hongchao Zhang's CG_DESCENT method in Chapter 3.

2.3 An Introduction Of CG_DESCENT Method

CG_DESCENT (refer to [1] and [4]) is a conjugate gradient method for solving an unconstrained optimization problem:

$$\min\{f(x) : x \in R^n\},$$

where $f : R^n \to R$ is continuously differentiable. The variable x_k satisfies the recurrence: $x_{k+1} = x_k + \alpha_k d_k$. α_k is the step size and is positive. d_k is called the searching direction. It's generated by the following rule:

(2.3.1) $$d_{k+1} = -g_{k+1} + \beta_k d_k, \quad d_0 = -g_0.$$

In CG_DESCENT method, a special choice for the parameter β_k was developed:

$$\beta_k = \max\{B_k, \eta_k\}, \text{ where } \eta_k = -\frac{1}{\|d_k\| \min\{\eta, \|g_k\|\}}, \text{ and}$$

$$B_k = \frac{1}{d_k^T y_k}(y_k - 2d_k \frac{\|y_k\|^2}{d_k^T y_k})^T g_{k+1}.$$

η is a positive constant and α_k is updated by a line search procedure. It uses secant and bisecant steps for faster convergence rate. This procedure will stop as soon as the Wolfe's conditions are satisfied. The Wolfe's conditions are:

(2.3.2) $$\delta\phi'(0) \geq \frac{\phi(\alpha_k) - \phi(0)}{\alpha_k} \text{ and } \phi'(\alpha_k) \geq \sigma\phi'(0),$$

where $\phi(\alpha) = f(x_k + \alpha d_k)$. Note that δ and σ are positive constants satisfying $0 < \delta \leq \sigma < 1$.

The disadvantage of using the Wolfe's condition is that when the variable x_k is close to the local minimum, the term $\phi(\alpha_k) - \phi(0)$ becomes relatively inaccurate. Hence, in [1], (2.3.2) is replaced by the approximate Wolfe conditions:

(2.3.3) $$(2\delta - 1)\phi'(0) \geq \phi'(\alpha_k) \geq \sigma\phi'(0),$$

where $0 < \delta < 1/2$ and $\delta \leq \sigma < 1$. This condition will be used only when the function value reaches some neighborhood of a local minimum.

By default, this method will apply approximate Wolfe condition. User can compute with the standard Wolfe conditions by setting AWolfe parameter to FALSE in the CG_DESCENT parameter file.

2.4 Applying CG_DESCENT In Optimal Control Problem

First we initialize the control variable $\{u(t_k)\}_{k=0}^n$: $u_0 = \{u_0(t_k)\}_{k=0}^n$. Then, we update the control by $u_{k+1} = u_k + \alpha_k d_k$, where α_k is the searching step size and d_k is the searching direction generated by (2.3.1). The step size α_k is computed with the same fashion as in Section 2.3. The updating of the controller will terminate if:

$$\left\|\nabla_u \phi(x_N)\right\| \leq \textit{gradient tolerance}.$$

This method has been implemented in C. The program is called OPTCON.C.

CHAPTER 3
IMPLEMENTATION OF OPTCON

3.1 Introduction Of OPTCON

OPTCON is a C program for solving the problems (1.0.1)-(1.0.3). It can be downloaded at http://www.math.ufl.edu/~lishuo/optcon.html.

In OPTCON, we provide the routine that evaluates the gradient $\nabla\widetilde{J}(u)$ and the routine that evaluates the objective cost $\widetilde{J}(u)$. The optimization is performed using Dr. Hager and Hongchao Zhang's CG_DESCENT. The main components of OPTCON are shown in Figure 3-1.

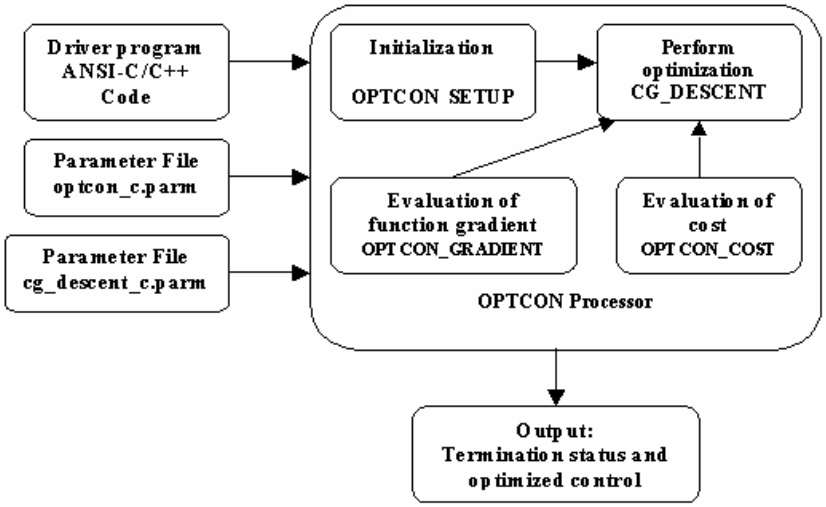

Figure 3-1. Main components of OPTCON

To use this program, user needs to provide a driver code, with the following routines:

- The routine that evaluates $\phi(x(t_f))$
- The routine that evaluates $\dfrac{d\phi}{dx}(x(t_f))$

- The routine that evaluates $f(x,u,t) \in R^{nx}$
- The routine that evaluates $\frac{\partial f}{\partial x}(x,u,t) \in R^{nx \times nx}$
- The routine that evaluates $\frac{\partial f}{\partial u}(x,u,t) \in R^{nx \times nc}$

How to use OPTCON package and the sample problems can be found in the Appendix A.

3.2 Comparison Of Performances

For evaluate the performance of OPTCON, we compare with another code GP.C, which uses the gradient projection method [5], with an Armijo rule for step and then applies the conjugate gradient method with Polak-Ribiere update of the search direction. The source code can be found and downloaded at:

http://www.math.ufl.edu/~lishuo/optcon.html.

We compare the performances using problem 1 and problem 2 in the Appendix A. Note that in these two codes we apply the same Runge-Kutta scheme, time mesh intervals, initial guess, and gradient tolerance. Since problem 2 is solved by penalty approach, we also apply the same penalty factor. The results are as follows:

Table 3-1. Comparison of performance for problem 1

Optimization method	Cost evaluation	Gradient evaluation	CG iterations	CPU time
CG_DESCENT Gradient Projection	32 times 170 times	34 times 170 times	20 47	0.11 sec. 0.24 sec.

Table 3-2. Comparison of performance for problem 2

Optimization method	Cost evaluation	Gradient evaluation	CG iterations	CPU time
CG_DESCENT Gradient Projection	2616 times 25815 times	3379 times 23947 times	1367 2736	18.00 sec. 139.00 sec.

It’s clear that OPTCON with the new CG_DESCENT method runs much faster than the previous conjugate gradient method.

CHAPTER 4
SURVEY AND ANALYSIS

This method can perform differently upon different choice of parameters and schemes. In this chapter, we will discuss performance relative to the parameters of CG_DESCENT and the Runge-Kutta schemes. Note that the sample problems we use in this Chapter can be found in Appendix A.

4.1 Penalty Factor

Let's use the problem 2 in Appendix A. We solve this problem by using a penalty approach. Since the problem provides the final-time boundary condition: $x_2(t_f) = 0$ and $x_3(t_f) = \sqrt{\frac{\mu}{x_1(t_f)}}$, we try to minimize the terms: $|x_2(t_N) - 0|$ and $\left| x_3(t_N) - \sqrt{\frac{\mu}{x_1(t_N)}} \right|$.

Hence, the target cost function becomes:

$$\begin{aligned} \tilde{J}(x_1, x_2, x_3, \theta, t) = -x_1(t_N) + P(x_2(t_N) - 0)^2 + P\left(x_3(t_N) - \sqrt{\frac{\mu}{x_1(t_N)}} \right)^2 \\ + \lambda_k^T \begin{pmatrix} x_2(t_N) \\ x_3(t_N) - \sqrt{\frac{\mu}{x_1(t_N)}} \end{pmatrix} \end{aligned} \quad (4.1.1)$$

where P is the penalty factor. The multiplier vector λ_k is updated by:

$$\lambda_{k+1} = \lambda_k + 2P \begin{pmatrix} x_2(t_N) \\ x_3(t_N) - \sqrt{\frac{\mu}{x_1(t_N)}} \end{pmatrix}. \quad (4.1.2)$$

We will recursively apply OPTCON, and update the multiplier vector λ_k in each iteration. Now, let's try different values of penalty factor. Table 4-1 shows the infinity

norm of the state error and the total CPU time for different choice of penalty factors. Note: we apply time mesh size $N = 500$, Runge-Kutta scheme 2 (see Table A-1 in Appendix A) and $grad\_tol = 10^{-5}$ for all iterations.

Table 4-1. Discrete state error in L^{∞} and CPU time with different penalty factors

Iterations	P = 1000	P = 5000	P = 10000	P = 50000	P = 500000
1	5.87e-003	1.43e-003	7.38e-004	1.52e-004	1.53e-005
2	1.52e-003	1.35e-004	3.84e-005	1.71e-006	1.76e-008
3	6.30e-004	1.66e-005	2.51e-006	2.37e-008	2.21e-011
4	2.59e-004	2.04e-006	1.64e-007	3.39e-010	3.61e-011
5	1.06e-004	2.49e-007	1.07e-008	1.78e-011	CPU time: 36 sec.
6	4.37e-005	3.05e-008	6.56e-010	3.49e-011	
7	1.79e-005	3.66e-009	9.49e-011	CPU time: 33 sec.	
8	7.37e-006	4.97e-010	2.33e-011		
9	3.03e-006	1.13e-010	2.33e-011		
10	1.24e-006	2.16e-011	CPU time: 27 sec.		
11	5.11e-007	1.78e-011			
12	2.10e-007	1.78e-011			
13	8.62e-008	CPU time: 20 sec.			
14	3.53e-008				
15	1.46e-008				
16	5.95e-009				
17	2.41e-009				
18	1.34e-009				
19	4.10e-010				
20	3.71e-010				
21	1.65e-010				
22	1.70e-010				
	CPU time: 14 sec.				

Greater penalty factor yields faster convergence rate. However, higher convergence rate is sacrificed with longer CPU time. Note that when you choose penalty factor P less than 1000, this method will not converge.

4.2 A Study Of The Gradient Tolerance Factor–c

For each of (4.1.2) we solve the discrete problem (4.1.1) to level of accuracy using CG_DESCENT. The convergence criterion in CG_DESCENT is based on the $\infty - norm$ of the gradient. The code terminates when this $\infty - norm$ is less than an input parameter *grad_tol*.

We apply $grad\_tol = 10^{-5}$ at the first iteration. Then, we compute the error $\|x(t_N) - x(t_f)\|_\infty$, and set $grad\_tol = c \cdot \|x(t_N) - x(t_f)\|_\infty$ for the next iteration. Table B-1 to Table B-9 in Appendix B provide the performance data when we choose different value of c. From these data, we obtain:

Table 4-2. Performance of OPTCON using different value of gradient tolerance factor

Factor c	CPU time	$\|x(t_N) - x(t_f)\|_\infty$	CG iterations
100,000	Unbounded		
10,000	20.00 sec.	4.47e-011	1693
1,000	22.00 sec.	6.76e-012	1917
100	24.00 sec.	2.36e-011	2119
10	29.00 sec.	2.53e-011	2578
1	31.00 sec.	2.63e-011	2548
0.1	35.00 sec.	9.18e-012	2842
0.01	36.00 sec.	3.17e-011	3053
0.001	36.00 sec.	3.17e-011	3053

Based on the total CPU time listed in Table 4-2, we obtained Figure 4-1:

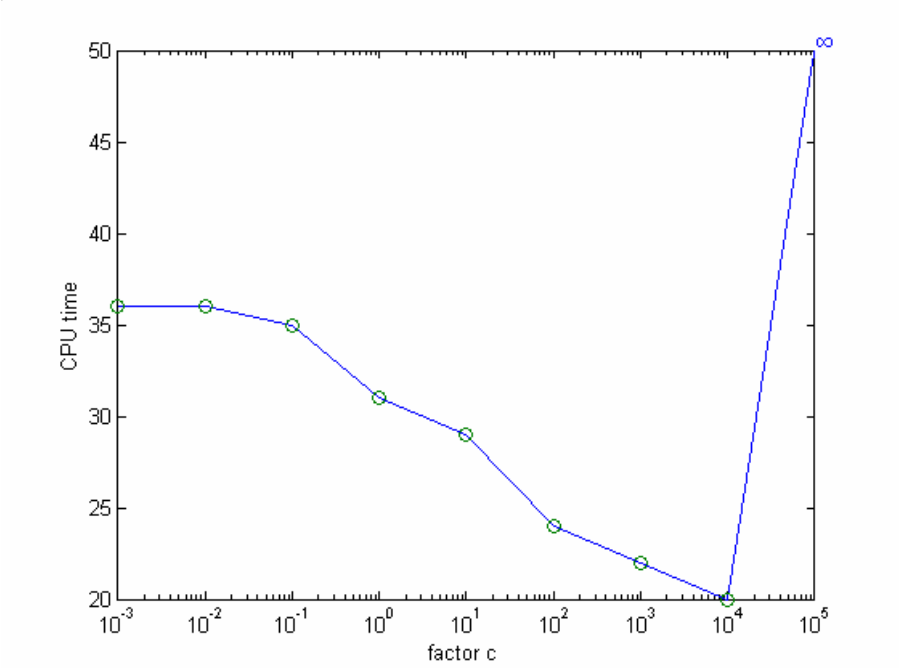

Figure 4-1. The relation of gradient tolerance factor *c* and CPU time

Comparing the performance with the different value of *c*, we can conclude that:

1. Very large *c* will not work. In this case, when $c = 100000$ the computation does not converge. CPU time $\to \infty$ as $c \geq 100000$.

2. Choosing smaller *c* can take longer CPU time.

3. The largest *c* such that computation converges provides the best CPU time.

4.3 A Study of Line Search Parameters

In the previous computation, we always used an approximate Wolfe line search [1]. Now, we will use a combination line search where the ordinary Wolfe conditions are used until the function value (4.1.1) average is sufficiently small. Then, we switch to approximate Wolfe conditions. To do this, we should set "AWolfe" parameter in CG_DESCENT_C.PARM to "FALSE". See Appendix B, Table B-10 to Table B-17. By these data we have:

Table 4-3. Performance of OPTCON using a combination line search conditions

Factor c	CPU time	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CG iterations
100,000	Unbounded		
10,000	15.00 sec.	5.17e-011	1279
1,000	18.00 sec.	2.33e-011	1453
100	21.00 sec.	2.11e-011	1758
10	23.00 sec.	2.27e-011	1843
1	26.00 sec.	4.08e-011	2224
0.1	29.00 sec.	2.76e-011	2401
0.01	30.00 sec.	4.25e-011	2406
0.001	30.00 sec.	4.25e-011	2406

Comparing the performance of OPTCON using combination line search conditions with the previous one, we get the following figure:

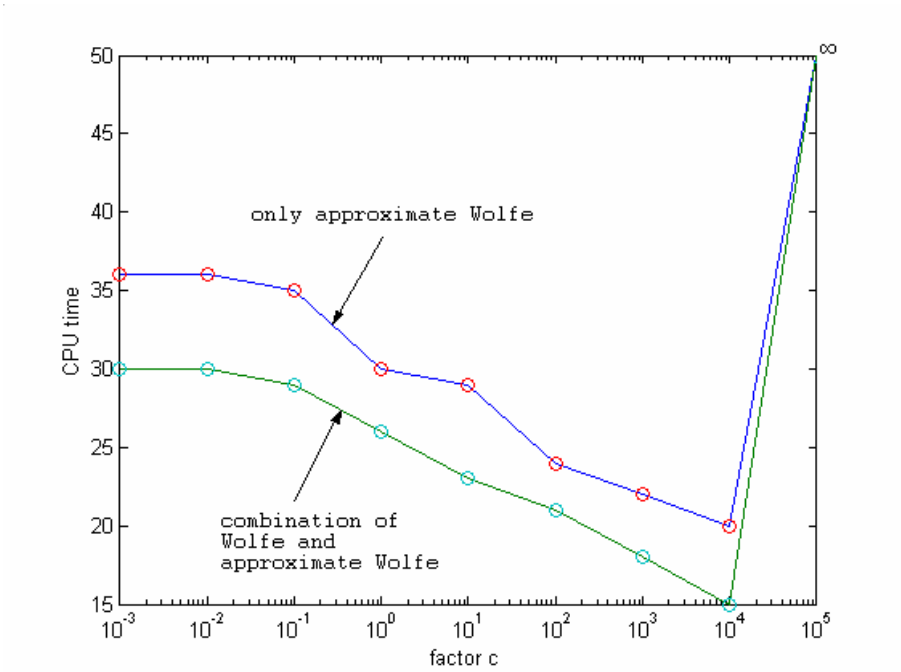

Figure 4-2. Comparison of CPU time when applying a combination of Wolfe/approximate Wolfe

It is clear that the performance is improved when we applying a combination line search. The best CPU time is 15 seconds, one fourth faster than the previous one.

4.4 Applying Different Runge-Kutta Schemes

OPTCON provides 6 optional explicit Runge-Kutta schemes (see Appendix A Table A-1). Using different schemes results in different performance. For problem 1 in

the Appendix A, the discrete state error in L^{∞} for different choice of Runge-Kutta schemes and different time mesh is shown in Table 4-4:

Table 4-4. Discrete state error in L^{∞} for test problem 1 and schemes 1-6

time mesh	Scheme 1	Scheme 2	Scheme 3	Scheme 4	Scheme 5	Scheme 6
N=2000	7.0e-008	8.0e-012	1.5e-008	3.5e-008	6.0e-008	1.4e-013
N=1000	2.8e-007	6.4e-011	6.1e-008	1.4e-007	2.4e-007	1.6e-013
N=600	7.8e-007	3.0e-010	1.7e-007	3.9e-007	6.7e-007	5.4e-013
N=320	2.7e-006	2.0e-009	5.9e-007	1.4e-006	2.4e-006	5.9e-012
N=160	1.1e-005	1.6e-008	2.4e-006	5.5e-006	9.5e-006	9.6e-011
N=80	4.4e-005	1.3e-007	9.7e-006	2.2e-005	3.8e-005	1.5e-009
N=40	1.8e-004	1.1e-006	3.9e-005	8.9e-005	1.6e-004	2.4e-008

Scheme 6 which has the fourth order of accuracy provides the best discretization error for this problem. Notice to obtain error on the order of 10^{-8}, we need to take N=2000, 160, 1000, 2000, 2000, 40 for schemes 1-6 respectively.

Table 4-5 shows the performance of Runge-Kutta schemes 1-6 applying to the problem 2 (Appendix A) with respect to $P = 10000$ and the corresponding N.

Table 4-5. Discrete state error in L^{∞} and CPU time for test problem 2 and schemes 1-6

	Scheme 1 N=2000	Scheme 2 N=160	Scheme 3 N=1000	Scheme 4 N=2000	Scheme 5 N=2000	Scheme 6 N=40
$\left\|x(t_N) - x(t_f)\right\|_{\infty}$	4.2e-011	7.4e-011	9.3e-012	2.6e-011	2.6e-011	7.6e-012
CPU time	27.00 sec	6.00 sec	69.00 sec	43.00 sec	65.00 sec	1.00 sec

It shows that scheme 6 provides the best CPU time. Among the third order schemes (schemes 2-5), scheme 2 gives the best performance.

APPENDIX A
HOW TO USE OPTCON

System Requirement

OPTCON uses GNU **gcc** complier, which is available on most UNIX systems. Availability of memories for running the program depends on the complexity of the problem. Once you run OPTCON, it will first check the availability of your computer memory.

Parameter File and Default Values

There are two parameter files in OPTCON package. One file is cg_descent_c.parm, which is used in CG_DESCENT. The meaning of the parameters and their default values can be found in [6]. Another parameter file optcon_c.parm is used in OPTCON subroutine. The parameters are the following:

1. PrintLevel-1 means print the result for each iteration, 0 means no print
2. PrintFinal-1 means print the final result, 0 means no print
3. scheme-choice of explicit Runge-Kutta schemes. (There are 6 options of schemes, see Table A-1) 0 means user defines his/her own Runge-Kutta scheme.

Table A-1. The six provided Runge-Kutta schemes

Scheme 1	Scheme 2
$A=\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}, b=\begin{pmatrix}1/2\\ 1/2\end{pmatrix}$	$A=\begin{pmatrix}0 & 0 & 0\\ 1/2 & 0 & 0\\ -1 & 2 & 0\end{pmatrix}, b=\begin{pmatrix}1/6\\ 2/3\\ 1/6\end{pmatrix}$
Scheme 3	**Scheme 4**
$A=\begin{pmatrix}0 & 0 & 0\\ 1/2 & 0 & 0\\ 0 & 3/4 & 0\end{pmatrix}, b=\begin{pmatrix}2/9\\ 1/3\\ 4/9\end{pmatrix}$	$A=\begin{pmatrix}0 & 0 & 0\\ 1/2 & 0 & 0\\ 1/2 & 1/2 & 0\end{pmatrix}, b=\begin{pmatrix}1/3\\ 1/3\\ 1/3\end{pmatrix}$
Scheme 5	**Scheme 6**
$A=\begin{pmatrix}0 & 0 & 0\\ 1 & 0 & 0\\ 1/4 & 1/4 & 0\end{pmatrix}, b=\begin{pmatrix}1/6\\ 1/6\\ 2/3\end{pmatrix}$	$A=\begin{pmatrix}0 & 0 & 0 & 0\\ 1/2 & 0 & 0 & 0\\ 0 & 1/2 & 0 & 0\\ 0 & 0 & 1 & 0\end{pmatrix}, b=\begin{pmatrix}1/6\\ 1/3\\ 1/3\\ 1/6\end{pmatrix}$

The default values of OPTCON parameters are:

Table A-2. Parameters' default values in optcon_c.parm

Parameter's name	Default value
PrintLevel	0
PrintFinal	1
scheme	2

Running OPTCON

To run the OPTCON, the user needs to create a driver program, which should be placed in the same directory where the OPTCON package stored. I will demonstrate how to use OPTCON with the following example.

Problem 1: (can be found in [1].)

(A1) minimize $\frac{1}{2}\int_0^1 u(t)^2 + 2x(t)^2 dt$

(A2) subject to $x'(t) = .5x(t) + u(t), x(0) = 1$

This problem can be solved with the analytic optimal solution:

$$x^*(t) = \frac{2e^{3t} + e^3}{e^{3t/2}(2 + e^3)}, \quad u^*(t) = \frac{2(e^{3t} - e^3)}{e^{3t/2}(2 + e^3)}.$$

Now, let $x(t)$ be denoted by $x_1(t)$ and $x_2'(t) = 2x_1(t)^2 + u(t)^2$, by fundamental theorem of calculus, the original cost function (A1) is equals to:

(A3) $$\text{minimize } \frac{1}{2}[x_2(1) - x_2(0)].$$

Let $x_2(0) = 0$, we transform the original problem into:

(A4) $$\text{minimize } \phi = \frac{1}{2}x_2(1)$$

(A5) $$\text{subject to } x_1'(t) = .5x_1(t) + u(t), x_1(0) = 1$$

(A6) $$x_2'(t) = 2x_1(t)^2 + u(t)^2, x_2(0) = 0.$$

Now, we create the driver program-driver1.c of the transformed system (A4)-(A6). Note that we use the default values of the OPTCON parameters.

```
#include "optcon.h"

double my_phi(double *x_f);
void my_dphi(double *dphi, double *x_f);
void my_f(double *f, double *x, double *u, double time);
void my_fx(double *fx, double *x, double *u, double time);
void my_fu(double *fu, double *x, double *u, double time);

int n = 500; // number of time mesh intervals
int nx = 2;  // number of state variables
int nc = 1;  // number of controls
int ns = 3;  // number of stage(s) in Runge-Kutta scheme

int main(void) {
       double t0, tf;
       double grad_tol = 1.0e-15;
       double *state0;
       double *state;
       double *control;
       double *a, *b; // Runge-Kutta matrix a and vector b
       int i;

       /* define initial time and final time */
       t0 = 0;
       tf = 1;

       /* allocate computer memory */
       state0 = (double*) malloc(nx*sizeof(double));
       state = (double*) malloc((n*ns*nx+nx)*sizeof(double));
       control = (double*) malloc(n*ns*nc*sizeof(double));

       /* guess of control */
       for ( i = 0; i < n*ns*nc; i ++ ) {
           control[i] = .5;
       }

       /* initial states */
       state0[0] = 1;
       state0[1] = 0;

       /* call OPTCON */
       optcon(grad_tol, n, nx, nc, ns, t0, tf, control, state0,
              state, a, b, my_phi, my_dphi, my_f, my_fx, my_fu);

       free(state0)
       free(state);
       free(control);
}
double my_phi(double *x_f) {
     return .5*x_f[1];
}
void my_dphi(double *dphi, double *x_f) {
     dphi[0] = 0;
     dphi[1] = .5;
     return;
}
void my_f(double *f, double *x, double *u, double time) {
     f[0] = .5*x[0] + u[0];
     f[1] = u[0]*u[0] + 2*x[0]*x[0];
     return;
}
void my_fx(double *fx, double *x, double *u, double time) {
     fx[0] = 0.5;
     fx[2] = 4*x[0];
     fx[1] = 0;
     fx[3] = 0;
     return;
}
void my_fu(double *fu, double *x, double *u, double time) {
     fu[0] = 1;
     fu[1] = 2*u[0];
     return;
}
```

Figure A-1. Driver1.c

Line 9 to 12 defined the number of time mesh intervals-*n*, number of state variables-*nx*, number of controls-*nc* and number of stage(s)-*ns* in the Runge-Kutta scheme. Note that the size of the state array is $n \times ns \times nx + nx$ (see line 29), in which the last nx elements store the final state. Let $x_{i,j}^k$ be the discrete state, where *k* is the time level $0 \le k \le n-1$, *i* is the component of state $1 \le i \le nx$, and *j* is the stage in Runge-Kutta scheme $1 \le j \le ns$. We store $x_{i,j}^k$ in the array state as the following:

For each fixed *j* and *k*, we first increment *i* from 1 to *nx*, next we increment *j* from 1 to *ns*, and finally we increment *k* from 0 to $n-1$. The discrete control $u_{i',j}^k$ $(1 \le i' \le nc)$ is stored in the control array (defined in line 30) in the same fashion. The user-provide routines include: (line 49 to 73 in Figure A-1)

- *double my_phi(double *x_f)* – the routine that evaluates the cost function $\phi(x(t_f))$. The input is "*double *x_f*"-a pointer points to the first element of the array *x_f* which contains the final states. Output is a double precision value of cost $\phi(x(t_f))$.

- *void my_dphi(double *dphi, double *x_f)* – the routine that evaluates $\frac{d\phi}{dx}(x(t_f))$. "*Double *x_f*" is input. Output is the array *dphi* that contains the value of $\frac{d\phi}{dx}(x(t_f)) \in R^{nx}$.

- *void my_f(double *f, double *x, double *u, double time)* – the routine that evaluates the system dynamic function $f(x,u,t) \in R^{nx}$. Inputs are: "*double *x*"-an array contains the states *x*, "*double *u*"-an array contains the controls *u*, and "*double time*"-time *t*. The output is "*double *f*"-an array contains the value of $f(x,u,t) \in R^{nx}$.

- *void my_fx(double *fx, double *x, double *u, double time)* – the routine that evaluates $\frac{\partial f}{\partial x}(x,u,t) \in R^{nx \times nx}$. "*Double *x*", "*double *u*", and "*double time*" are inputs. The output is "double **fx*"-an array contains the value of $\frac{\partial f}{\partial x}(x,u,t) \in R^{nx \times nx}$. Note that we store the matrix by rows (line 63-66).

- void my_fu(double *fu, double *x, double *u, double time) – the routine that evaluates $\frac{\partial f}{\partial u}(x,u,t) \in R^{nx \times nc}$. "*Double *x*", "*double *u*", and "*double time*" are inputs. The output is "*double *fu*"-an array contains the value of $\frac{\partial f}{\partial u}(x,u,t) \in R^{nx \times nc}$. Note that we store the matrix by rows (line 70 and 71).

We applied the provided Runge-Kutta scheme in this example. To provide your own Runge-Kutta scheme, you should set the "scheme" parameter to 0 and initialize the *a* and *b* arrays (line 20) to contain the coefficients of the scheme (as shown in Figure A-2, line 20, 21). Note that we store the coefficients of Runge-Kutta matrix A by rows.

Suppose the user-provide Runge-Kutta matrix A and vector b are: $A=\begin{pmatrix} 0 & 0 & 0 \\ .5 & 0 & 0 \\ .5 & .5 & 0 \end{pmatrix}$, $b=\begin{pmatrix} 1/3 \\ 1/3 \\ 1/3 \end{pmatrix}$

```
14      int main(void) {
15              double t0, tf;
16              double grad_tol = 1.0e-15;
17              double *state0;
18              double *state;
19              double *control;
20              double a[9] = {0, 0, 0, .5, 0, 0, .5, .5, 0}; // Runge-Kutta matrix a
21              double b[3] = {1./3., 1./3., 1./3.}; // Runge-Kutta vector b
22              int i;
23
24              /* define initial time and final time */
25              t0 = 0;
26              tf = 1;
27
28              /* allocate computer memory */
29              state0 = (double*) malloc(nx*sizeof(double));
30              state = (double*) malloc((n*ns*nx+nx)*sizeof(double));
31              control = (double*) malloc(n*ns*nc*sizeof(double));
32
33              /* guess of control */
34              for ( i = 0; i < n*ns*nc; i ++ ) {
35                  control[i] = .5;
36              }
37
38              /* initial states */
39              state0[0] = 1;
40              state0[1] = 0;
41
42              /* call OPTCON */
43              optcon(grad_tol, n, nx, nc, ns, t0, tf, control, state0,
44                      state, a, b, my_phi, my_dphi, my_f, my_fx, my_fu);
45
46              free(state0)
47              free(state);
48              free(control);
49      }
```

Figure A-2. Segment of Driver1.c for the case that user provides Runge-Kutta scheme

After calling OPTCON (line 42 in Figure A-1 or line 43 in Figure A-2), we obtain the final state (the last nx elements in the state array) and the discrete optimal control for problem 1.

Now, let's consider another example, which has both initial conditions and final conditions.

Problem 2: orbit transfer problem (see [7] page 66-68).

For a constant-thrust rocket with thrust T, operating from time 0 to time t_f, we want to find an optimal thrust angle history $\theta(t)$ that transfer the rocket from an initial given orbit to the largest possible circular orbit. Now, let's transform it into a mathematical model. First, the variables and parameters are given by: x_1-the radius of the orbit with an attracting center; x_2-the radial velocity; x_3-the tangential velocity; m_0-the mass of the rocket; $\dot{m}$-the fuel consumption rate; $\theta(t)$-the history of thrust angle; μ-the gravity constant of the attracting center. Then, the model is formulated by:

(A7) maximize $x_1(t_f)$,

System dynamics:

(A8) $$x_1' = x_2,$$

(A9) $$x_2' = \frac{{x_3}^2}{x_1} - \frac{\mu}{{x_1}^2} + \frac{T\sin\theta}{m_0 - |\dot{m}|t},$$

(A10) $$x_3' = -\frac{x_2 x_3}{x_1} + \frac{T\cos\theta}{m_0 - |\dot{m}|t}.$$

Initial conditions:

(A11) $$x_1(0) = a,$$

(A12) $$x_2(0) = 0,$$

(A13) $$x_3(0) = \sqrt{\frac{\mu}{a}}.$$

Final conditions:

(A14) $$x_2(t_f) = 0,$$

(A15) $$x_3(t_f) = \sqrt{\frac{\mu}{x_1(t_f)}}.$$

Where, $m_0 = 10{,}000kg, \dot{m} = 12.9kg/day, a = 149.6\times10^9 m, T = 8.336N,$

$\mu = 1.3273310^{20} m^3/s^2$ and $t_f = 193days$.

Since the final conditions are given, we solve this problem using a penalty approach. At step *k*, the cost function is given by:

(A16)
$$\phi(x_1(t_N), x_2(t_N), x_3(t_N)) = -x_1(t_N) + Px_2(t_N)^2 + P\left(x_3(t_N) - \sqrt{\frac{\mu}{x_1(t_N)}}\right)^2 + \lambda_{1,k}x_2(t_N) + \lambda_{2,k}\left(x_3(t_N) - \sqrt{\frac{\mu}{x_1(t_N)}}\right)$$

with Lagrange multipliers λ_1 and λ_2, and a constant penalty factor P. At step $k+1$, λ_1 and λ_2 are updated by:

(A17) $$\lambda_{1,k+1} = \lambda_{1,k} + 2Px_2(t_N),$$

(A18) $$\lambda_{2,k+1} = \lambda_{2,k} + 2P\left(x_3(t_N) - \sqrt{\frac{\mu}{x_1(t_N)}}\right).$$

Note that $\lambda_{1,0}$ and $\lambda_{2,0}$ are given.

By penalty approach, we solve this problem by recursively calling OPTCON, each iteration involved in updating the value of λ_1 and λ_2. The program will stop when the

value $\left|x_2(t_N)\right| + \left|x_3(t_N) - \sqrt{\frac{\mu}{x_1(t_N)}}\right|$ is no longer decreasing. Please refer to the driver program-driver2.c, which can be found in the OPTCON package.

APPENDIX B
TESTING DATA FOR GRADIENT TOLERANCE FACTOR

We test different value of gradient tolerance factor *c* for problem 2 in Appendix A. Let's apply time mesh size $N = 500$, scheme 2 (see Table A-1 in Appendix A), penalty factor $P = 10000$, and initial $grad\_tol = 10^{-5}$.

Using only approximate Wolfe line search conditions in CG_DESCENT, we obtain Table B-1 to Table B-9.

Table B-1. Performance of OPTCON when gradient tolerance factor $c = 100000$

Iteration #	$\|x(t_N) - x(t_f)\|_\infty$	CPU time	CG iterations
1	4.54e-004	11.00 sec	1128
2	7.44e-005	0.00 sec	2
3	3.80e-005	0.00 sec	6
4	5.48e-006	1.00 sec	12
5	9.31e-006	0.00 sec	39
		Not convergent	

Table B-2. Performance of OPTCON when gradient tolerance factor $c = 10000$

Iteration #	$\|x(t_N) - x(t_f)\|_\infty$	CPU time	CG iterations
1	4.54e-004	12.00 sec	1128
2	4.24e-005	0.00 sec	22
3	1.02e-005	0.00 sec	28
4	5.21e-007	0.00 sec	26
5	6.42e-008	1.00 sec	66
6	3.20e-009	1.00 sec	35
7	4.98e-010	1.00 sec	136
8	1.06e-010	1.00 sec	60
9	7.25e-011	1.00 sec	49
10	2.58e-011	2.00 sec	120
11	1.50e-011	0.00 sec	4
12	3.91e-012	1.00 sec	18
13	4.47e-011	0.00 sec	1
		Total: 20.00 sec	

Table B-3. Performance of OPTCON when gradient tolerance factor $c = 1000$

Iteration #	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CPU time	CG iterations
1	4.54e-004	12.00 sec	1128
2	2.89e-005	0.00 sec	80
3	2.58e-006	2.00 sec	91
4	2.42e-007	0.00 sec	82
5	1.88e-008	2.00 sec	114
6	1.00e-009	1.00 sec	109
7	8.39e-011	1.00 sec	97
8	4.60e-011	3.00 sec	184
9	1.27e-011	1.00 sec	9
10	5.80e-012	0.00 sec	7
11	6.76e-012	0.00 sec	16
		Total: 22.00 sec	

Table B-4. Performance of OPTCON when gradient tolerance factor $c = 100$

Iteration #	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CPU time	CG iterations
1	4.54e-004	11.00 sec	1128
2	2.95e-005	2.00 sec	133
3	2.04e-006	2.00 sec	138
4	1.35e-007	1.00 sec	132
5	8.95e-009	3.00 sec	288
6	5.95e-010	3.00 sec	231
7	7.19e-011	1.00 sec	33
8	1.10e-011	1.00 sec	21
9	2.36e-011	0.00 sec	15
		Total: 24.00 sec	

Table B-5. Performance of OPTCON when gradient tolerance factor $c = 10$

Iteration #	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CPU time	CG iterations
1	4.54e-004	12.00 sec	1128
2	2.96e-005	2.00 sec	172
3	1.92e-006	2.00 sec	208
4	1.26e-007	3.00 sec	294
5	8.19e-009	5.00 sec	410
6	5.51e-010	2.00 sec	171
7	8.01e-011	0.00 sec	27
8	2.03e-011	1.00 sec	51
9	7.67e-012	1.00 sec	87
10	2.53e-011	1.00 sec	30
		Total: 29.00 sec	

Table B-6. Performance of OPTCON when gradient tolerance factor $c = 1$

Iteration #	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CPU time	CG iterations
1	4.54e-004	12.00 sec	1128
2	2.96e-005	3.00 sec	246
3	1.93e-006	4.00 sec	342
4	1.26e-007	5.00 sec	355
5	8.25e-009	2.00 sec	175
6	5.22e-010	2.00 sec	114
7	3.65e-011	1.00 sec	88
8	1.09e-011	1.00 sec	97
9	4.12e-012	1.00 sec	1
10	2.63e-011	0.00 sec	2
		Total: 31.00 sec	

Table B-7. Performance of OPTCON when gradient tolerance factor $c = 0.1$

Iteration #	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CPU time	CG iterations
1	4.54e-004	12.00 sec	1128
2	2.96e-005	4.00 sec	350
3	1.93e-006	5.00 sec	377
4	1.26e-007	4.00 sec	363
5	8.17e-009	4.00 sec	258
6	5.52e-010	2.00 sec	150
7	9.22e-011	0.00 sec	52
8	4.66e-011	1.00 sec	37
9	3.65e-011	2.00 sec	76
10	1.54e-011	0.00 sec	2
11	1.32e-011	0.00 sec	10
12	6.47e-012	1.00 sec	19
13	9.18e-012	0.00 sec	20
		Total: 35.00 sec	

Table B-8. Performance of OPTCON when gradient tolerance factor $c = 0.01$

Iteration #	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CPU time	CG iterations
1	4.54e-004	11.00 sec	1128
2	2.96e-005	6.00 sec	441
3	1.93e-006	4.00 sec	404
4	1.26e-007	4.00 sec	327
5	8.21e-009	5.00 sec	378
6	5.16e-010	3.00 sec	200
7	7.05e-011	0.00 sec	48
8	2.31e-011	2.00 sec	104
9	3.17e-011	1.00 sec	23
		Total: 36.00 sec	

Table B-9. Performance of OPTCON when gradient tolerance factor $c = 0.001$

Iteration #	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CPU time	CG iterations
1	4.54e-004	11.00 sec	1128
2	2.96e-005	5.00 sec	441
3	1.93e-006	5.00 sec	404
4	1.26e-007	4.00 sec	327
5	8.21e-009	5.00 sec	378
6	5.16e-010	3.00 sec	200
7	7.05e-011	0.00 sec	48
8	2.31e-011	2.00 sec	104
9	3.17e-011	1.00 sec	23
		Total: 36.00 sec	

Using a combination of Wolfe and approximate Wolfe line search conditions in CG_DESCENT, we obtain Table B-10 to Table B-17.

Table B-10. Performance of OPTCON using a combination line search, $c = 10000$

Iteration #	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CPU time	CG iterations
1	4.54e-004	8.00 sec	807
2	4.25e-005	0.00 sec	22
3	1.00e-005	1.00 sec	31
4	8.34e-007	0.00 sec	26
5	5.21e-008	1.00 sec	48
6	1.58e-008	1.00 sec	59
7	1.99e-010	0.00 sec	51
8	6.55e-011	2.00 sec	138
9	4.86e-011	1.00 sec	74
10	4.79e-011	0.00 sec	3
11	5.17e-011	1.00 sec	20
		Total: 15.00 sec	

Table B-11. Performance of OPTCON using a combination line search, $c = 1000$

Iteration #	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CPU time	CG iterations
1	4.54e-004	8.00 sec	807
2	2.82e-005	1.00 sec	71
3	3.36e-006	1.00 sec	79
4	1.15e-007	1.00 sec	60
5	9.48e-009	2.00 sec	132
6	8.46e-010	1.00 sec	95
7	4.25e-011	2.00 sec	114
8	2.35e-011	0.00 sec	34
9	1.70e-011	1.00 sec	15
10	2.33e-011	1.00 sec	46
		Total: 18.00 sec	

Table B-12. Performance of OPTCON using a combination line search, $c = 100$

Iteration #	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CPU time	CG iterations
1	4.54e-004	8.00 sec	807
2	2.97e-005	1.00 sec	138
3	1.83e-006	2.00 sec	140
4	1.26e-007	1.00 sec	129
5	7.74e-009	4.00 sec	314
6	4.82e-010	1.00 sec	82
7	6.55e-011	1.00 sec	50
8	9.31e-012	1.00 sec	83
9	2.11e-011	1.00 sec	15
		Total: 21.00 sec	

Table B-13. Performance of OPTCON using a combination line search, $c = 10$

Iteration #	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CPU time	CG iterations
1	4.54e-004	8.00 sec	807
2	2.96e-005	2.00 sec	181
3	1.92e-006	2.00 sec	184
4	1.26e-007	3.00 sec	234
5	8.23e-009	3.00 sec	250
6	5.04e-010	2.00 sec	139
7	6.21e-011	1.00 sec	28
8	6.92e-012	0.00 sec	17
9	2.27e-011	1.00 sec	3
		Total: 23.00 sec	

Table B-14. Performance of OPTCON using a combination line search, $c = 1$

Iteration #	$\|x(t_N) - x(t_f)\|_\infty$	CPU time	CG iterations
1	4.54e-004	8.00 sec	807
2	2.96e-005	2.00 sec	233
3	1.93e-006	4.00 sec	306
4	1.26e-007	4.00 sec	373
5	8.19e-009	3.00 sec	240
6	5.62e-010	3.00 sec	180
7	3.74e-011	1.00 sec	80
8	4.08e-011	1.00 sec	5
		Total: 26.00 sec	

Table B-15. Performance of OPTCON using a combination line search, $c = 0.1$

Iteration #	$\|x(t_N) - x(t_f)\|_\infty$	CPU time	CG iterations
1	4.54e-004	8.00 sec	807
2	2.96e-005	4.00 sec	358
3	1.93e-006	5.00 sec	368
4	1.26e-007	3.00 sec	275
5	8.23e-009	3.00 sec	237
6	5.32e-010	3.00 sec	165
7	4.86e-011	0.00 sec	44
8	1.68e-011	2.00 sec	97
9	1.52e-011	0.00 sec	5
10	2.76e-011	1.00 sec	45
		Total: 29.00 sec	

Table B-16. Performance of OPTCON using a combination line search, $c = 0.01$

Iteration #	$\|x(t_N) - x(t_f)\|_\infty$	CPU time	CG iterations
1	4.54e-004	8.00 sec	807
2	2.96e-005	6.00 sec	432
3	1.93e-006	5.00 sec	354
4	1.26e-007	3.00 sec	260
5	8.20e-009	4.00 sec	320
6	5.40e-010	2.00 sec	132
7	3.97e-011	1.00 sec	55
8	2.51e-011	1.00 sec	20
9	4.25e-011	0.00 sec	26
		Total: 30.00 sec	

Table B-17. Performance of OPTCON using a combination line search, $c = 0.001$

Iteration #	$\left\|x(t_N) - x(t_f)\right\|_\infty$	CPU time	CG iterations
1	4.54e-004	8.00 sec	807
2	2.96e-005	6.00 sec	432
3	1.93e-006	4.00 sec	354
4	1.26e-007	4.00 sec	260
5	8.20e-009	4.00 sec	320
6	5.40e-010	2.00 sec	132
7	3.97e-011	1.00 sec	55
8	2.51e-011	1.00 sec	20
9	4.25e-011	0.00 sec	26
		Total: 30.00 sec	

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