

Fall, 2017

06-606

COMPUTATIONAL METHODS FOR PROCESS ENGINEERING

Instructor: L.T. Biegler, DH 1111, 8-2232, lb01@andrew.cmu.edu
Time and Place: T, Th 3:30 – 5:20 PM, 4201 DH
Teaching Assistant: Saif Kazi, DH 3106, 8-2228, srkazi@andrew
Web Site: <http://numero.cheme.cmu.edu/course/06606.html>

The goal of this course is to cover methods for solution and optimization for engineering systems described by nonlinear algebraic and/or differential equations. The course will deal with solution strategies and nonlinear programming methods, and some properties of Differential/Algebraic systems. Applications will concentrate on process engineering as well as mechanical and nonlinear control systems. Course assignments will involve a modest amount of programming in FORTRAN or MATLAB, use of GAMS, NETLIB and other software.

<u>Week</u>	<u>Topic</u>
8/29, 31	Introduction; Math Models for Process Engineering, Course Overview
9/5, 7	Solution of Linear Algebraic Equations and Sparse Methods
9/12, 14	Solution of Nonlinear Algebraic Equations and quasi-Newton Methods
9/19, 21	Solution of ODE's by Runge-Kutta and Linear Multistep Methods
9/26, 28	Stability of ODE Solvers
10/3, 5	Introduction to DAE Systems, Solution of DAEs
10/10, 12	Project Proposal Due, Reduction of High Index Problems
10/17, 19	Review, Exam I
10/24	Solution of Boundary Value Problems, Collocation and Mesh Adaptation
11/3*	Sensitivity Analysis of DAE Systems, Direct Methods, Adjoint Methods
11/7, 9	Nonlinear Programming Concepts, Algorithms
11/14, 16	Optimization of DAE Systems, Background
11/21	Simultaneous Methods for Optimization of DAE Models
11/28, 30	Review, Exam II
12/5, 7	Extensions to Large-Scale Problems, Projects Due *Make-up classes will meet 8:30am – 10am in DH 4201

Computational Methods for Process Engineering

Course Grading and Assignments

Seven homework sets (plus one for extra credit) will be assigned at regular intervals over the course and posted on the course website. In addition, a course project is due at the end of the course involving a nontrivial application of DAE modeling and optimization. Course grading will consist of the following components.

Exam I (10/19)	30%
Exam II (11/28)	30%
Project	20 %
Homework	20%

Due dates: HW1 - 9/12/2017; HW2 - 9/21/2017; HW3 - 10/5/2017; HW4 - 10/17/2017;
 HW5 - 11/7/2017; HW6 - 11/16/2017; HW7 - 11/28/2017
 Extra Credit: HW8 - 12/7/2017 (worth 10 exam points)

Below is an initial list of reference books of background material in the E&S Library. Most of the material will be taken from the first and third texts (can be purchased on-line from <http://www.siam.org>). In addition, supporting material is on the course website. More specific sources dealing with applications or specialized strategies will be given later in the course as appropriate.

- Ascher, U. M., and L. R. Petzold, Computer Methods for Ordinary Differential Equations and Differential Algebraic Equations, SIAM, Philadelphia (1998)
- Ascher, U.M., R.M. Mattheij and R.D. Russell, Numerical Solution of Boundary Value Problems for Ordinary Differential Equations, Prentice-Hall, Englewood Cliffs, NJ (1988)
- Biegler, L. T., Nonlinear Programming: Concepts, Algorithms and Applications to Chemical Processes, SIAM, Philadelphia (2010)
- Biegler, L. T., I. E. Grossmann and A. W. Westerberg, Systematic Methods of Chemical Process Design, Prentice-Hall, Englewood Cliffs, NJ (1997)
- Brenan, K.E., S.L. Campbell and L.R. Petzold, Numerical Solution of Initial Value Problems in Differential-Algebraic Equations, North Holland, New York (1989)
- Bryson, A.E. and Y.C. Ho, Applied Optimal Control, Ginn/Blaisdell, New York, 1968.
- Dennis, J.E. and R.B. Schnabel, Numerical Methods for Unconstrained Optimization and Nonlinear Equations, Prentice-Hall, Englewood Cliffs, NJ (1986)
- Finlayson, B.A., Applied Nonlinear Analysis in Chemical Engineering, McGraw-Hill, 1980.
- Fletcher, R., Practical Methods of Optimization, Wiley, 1987.
- Nocedal, J. and S. Wright, Numerical Optimization, Springer, 1999
- Dianne P. O'Leary, Scientific Computing with Case Studies, SIAM, Philadelphia, 2009
- Phillips, G. M. and P. J. Taylor, Theory and Applications of Numerical Analysis, Academic Press, second edition, London (1996)