Fall, 2016 **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:	David Thierry, DH 3106, 8-2228, domolinat@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.

Week	Topic
8/30, 2*	Introduction; Math Models for Process Engineering, Course Overview
9/6, 8	Solution of Linear Algebraic Equations and Sparse Methods
9/13, 15	Solution of Nonlinear Algebraic Equations and quasi-Newton Methods
9/20	Solution of ODE's by Runge-Kutta and Linear Multistep Methods
9/27, 29*	Stability of ODE Solvers
10/4, 6	Review, Exam I
10/11, 13	Project Proposal Due, Introduction to DAE Systems
10/18, 20	Solution of DAEs, Reduction of High Index Problems
10/25, 27	Solution of Boundary Value Problems, Collocation and Mesh Adaptation
11/3	Sensitivity Analysis of DAE Systems, Direct Methods, Adjoint Methods
11/8, 10	Nonlinear Programming Concepts, Algorithms
11/15, 17	Review, Exam II
11/22	Optimization of DAE Systems, Background
11/29, 12/1	Simultaneous Methods for Optimization of DAE Models
12/6, 8	Extensions to Large-Scale Problems, Projects Due

*Make-up classes will meet 8:30am – 10am in DH 4201

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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	30%
Exam II	30%
Project	20 %
Homework	20%

Due dates: HW1 - 9/13/2016; HW2 - 9/22/2016; HW3 - 10/6/2016; HW4 - 10/25/2016; HW5 - 11/8/2016; HW6 - 11/17/2016; HW7 - 11/29/2016

Extra Credit: HW8 - 12/8/2016 (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)