Spring, 2020 **06-606**

COMPUTATIONAL METHODS FOR PROCESS ENGINEERING

Instructor: L.T. Biegler, DH 1111, 8-2232, lb01@andrew.cmu.edu

Time and Place: T, Th 3:00 – 4:20 PM, 4201 DH

Teaching Assistant: Kuan-han Lin, DH 4200, kuanhanl@andrew.cmu.edu

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 MATLAB or Python, use of GAMS and other software.

Week	Topic
1/14, 16	Course Overview, Math Models for Process Engineering
1/23	Solution of Linear Algebraic Equations and Sparse Methods
1/28, 30	Solution of Nonlinear Algebraic Equations and quasi-Newton Methods
2/4	Solution of ODE's by Runge-Kutta and Linear Multistep Methods
2/11, 13	Stability of ODE Solvers
2/18, 20	Introduction to DAE Systems, Solution of DAEs
2/25, 28*	Project Proposal Due, Reduction of High Index Problems *make-up class, DH 4201, 10:30 –12:30 pm
3/3, 5	Review, Exam I
3/19, 20*	Solution of Boundary Value Problems, Finite Differences and Collocation *make-up class, DH 4201, 10:30 –12:30 pm
3/24, 26	Sensitivity Analysis of DAE Systems, Direct Methods, Adjoint Methods
3/31, 4/2	Nonlinear Programming Concepts, Algorithms
4/7, 9	Optimization of DAE Systems, Background
4/14, 16	Simultaneous Methods for Optimization of DAE Models
4/21, 23	Review, Exam II
4/28, 30	Extensions to Large-Scale Problems, Projects Due

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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 (3/5)	30%
Exam II (4/23)	30%
Project (5/1)	20%
Homework	20%

Due dates: HW1 – 1/30; HW2 – 2/11; HW3 – 2/20; HW4 - 3/3; HW5 - 3/26; HW6 – 4/9; HW7 – 4/21
Extra Credit: HW8 – 5/1 (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)