COURSE OFFERING ON NUMERICAL METHODS

FINITE ELEMENT ANALYSIS IN CHEMICAL ENGINEERING:

WITH EMPHASIS ON

SOLUTION OF FREE BOUNDARY PROBLEMS IN FLUID MECHANICS, HEAT AND MASS TRANSFER, AND REACTION ENGINEERING

CHEMICAL ENGINEERING 697
SPRING SEMESTER 2014
Time: MWF 3:30-4:20 PM; Location: FRNY G124

INSTRUCTOR: PROF. OSMAN A. BASARAN
SCHOOL OF CHEMICAL ENGINEERING (OFFICE: FRNY 3060)
765-494-4061 (phone); 765-494-0805 (fax); obasaran@purdue.edu

---

Course philosophy and objectives. Over the last several decades, finite element methods have emerged as the numerical method of choice in diverse applications in which the equations that govern the transport of momentum, heat, and species have to be solved and/or free boundaries abound. Some well known applications of the finite element method to these problems have included free surface flows encountered in coating flows, polymer processing, and drop and bubble dynamics; porous media flows such as ones studied in ground water hydrology and contaminant transport; and solidification and phase change problems such as ones solved in analyses of crystal growth and chemical vapor deposition. This course will emphasize (but not be restricted to) the fundamentals and applications of the finite element method to nonlinear free boundary problems. This course supplements the fine selection of other courses on finite element methods that are offered at Purdue University by focusing on situations in which fluid-fluid and fluid-solid interfaces play a dominant role.

Course outline. The course will cover most of the following topics (coverage varies slightly from year to year), beginning with the fundamentals and then quickly moving on to apply the methods to certain problems at the frontiers of research.

Finite elements: one-, two-, and three-dimensional linear and nonlinear, steady and time-dependent problems; basis functions; ordinary and partial differential equations; integral equations; direct and iterative matrix solvers; automatic and adaptive mesh generation, and moving elements.

Stability analysis: turning and bifurcation points.

Applications. Examples from:

- capillary hydrostatics and solutions of the Young-Laplace equation;
- flows governed by the Navier-Stokes and the Euler equations, mixed-interpolation

and penalty methods;
- free surface flows — algebraic and elliptic mesh generation, drop dynamics, film and coating flows, and flows with interface rupture;
- flows with heat, mass, and charge transport — surface tension gradient-driven flows, electrohydrodynamics (i.e. coupled solution of the Cauchy momentum and Maxwell's equations), and flows encountered in the processing of electronic materials;
- polymer processing, rheology, and non-Newtonian fluid mechanics.

Other methods: survey of boundary element or boundary integral, finite difference, volume of fluid, level set, boundary collocation, and perturbation methods.

Instructional method. Extensive handouts of lecture notes and supplementary materials, algorithms, and computer programs. Homework (including writing of computer programs), test(s), and project. The latter may be open-ended and lead to publications and/or inclusion in M.S./Ph.D. theses. By the end of the course, participants will be able to read the research literature and use finite elements in their research/work. In past years, a small number of lectures on a hot or specialized topic has also been presented by an expert on that topic. This year, a number of such hot topical areas may once again be covered by several outside experts. These special lectures will be announced during the course of the semester.

Prerequisites. Class participants either should be familiar with or willing to learn during the course of the semester (a) using computers and FORTRAN, C, or some other high-level programming language (MATLAB is also acceptable), (b) vector and tensor analysis at the level of Chapter 6 of Hildebrand's *Advanced Calculus for Applications* and Appendix A of Bird, Stewart, and Lightfoot's *Transport Phenomena* (BSL), and (c) basics of transport phenomena at the level of BSL. A good background in calculus and ordinary and partial differential equations will also be helpful but no previous knowledge of numerical methods will be assumed.

Required and/or supplementary texts. Although there are no required textbooks this year, the following two books were required in recent offerings of this course.

1. M. S. Gockenbach, *Understanding and Implementing the Finite Element Method*, SIAM (2006).

2. W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes*, Cambridge U. Press (2007).

Moreover, the following books are highly recommended as general supplementary texts:

(i) G. Strang and G. J. Fix, *An Analysis of the Finite Element Method*, Prentice-Hall (1973). [The second edition of this classic, which was published in 2008, has a new part II that focuses on implementation issues.]

(ii) J. N. Reddy and D. K. Gartling, *The Finite Element Method in Heat Transfer and*

Fluid Dynamics, CRC Press (1994). [The third edition of this book was published in 2010. I do not recommend this book as a textbook from which one can learn finite elements.]

(iii) L. Lapidus and G. F. Pinder, *Numerical Solution of Partial Differential Equations in Science and Engineering*, Wiley-Interscience (1982).

For most of the material to be presented in the course, there are no appropriate texts. Therefore, lecture notes and handouts will be used in lieu of text during the course of the semester. A list of additional supplementary (reference) texts will be given out in class.

Course history. This course has its roots in a seminar/course taught by the instructor and his colleagues while he was a graduate student in the Department of Chemical Engineering and Materials Science at the University of Minnesota. Since that time, the scope of the course has greatly broadened. In particular, the course being offered is a direct offshoot of a graduate level course which was taught by the instructor biennially over a period of several years at the University of Tennessee and the Oak Ridge National Laboratory. The course was previously taught at Purdue University during Spring semesters 1996-8, 2002-3, 2006-9, and 2012-3.