

Course Syllabus

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CHE/BSE/BEAM 5044: Engineering Mathematics

Syllabus and Course Outline

Fall 2016

Days/Time: MWF 11:15am - 12:05pm

Location: Goodwin 115

Instructor: Ryan S. Senger

Department: Biological Systems Engineering

Office: 301C HABB1

Office Phone: 540-231-9501

Email: senger@vt.edu

Office Hours: Friday, 3-5pm

Course (Catalog) Description:

5984: Engineering Mathematics: This is an introduction to both the closed-form solution and numerical solution of partial differential equations with direct relevance to chemical engineering, biological systems engineering, and biomedical engineering and sciences. The instructor may cover additional topics such as numerical solution of ordinary differential equations, optimization, and data analysis when time permits.

Prerequisites: The minimum requirements are undergraduate mathematics, namely one year of calculus, exposure to ordinary differential equations, linear algebra and general familiarity with desktop computing. A student without an undergraduate degree in engineering should meet with the instructor before signing up for this course. The instructor will determine eligibility.

Textbooks: None required. (Optional) Pozrikidis, C. (2005) Introduction to Finite and Spectral Element Methods using Matlab.

Software:

MATLAB – Obtain through [Student Software Distribution \(http://www2.ita.vt.edu/software/student/products/mathworks/matlab/index.html\)](http://www2.ita.vt.edu/software/student/products/mathworks/matlab/index.html) (<http://www2.ita.vt.edu/software/student/>)

For more information on obtaining MATLAB, click [here \(http://www2.ita.vt.edu/software/student/products/mathworks/matlab/index.html\)](http://www2.ita.vt.edu/software/student/products/mathworks/matlab/index.html)

COMSOL – Available at the [Math Emporium \(http://www.emporium.vt.edu\)](http://www.emporium.vt.edu)

Course Objectives: At the conclusion of this course, students will be competent with the following topics. Application examples will be drawn from chemical engineering, biological systems engineering and biomedical engineering and sciences.

1. Basic MATLAB programming for building and parsing datasets
2. Numerical simulation of a system of ODEs

3. Gradient-based and evolutionary methods of optimization
4. Closed-form solutions of simple PDE models,
5. Finite element methods in one-, two-, and three-dimensions
6. Meshing and matrix assembly
7. Numerical simulations of two- and three-dimensional PDEs obtained using COMSOL

Evaluation and Grading

| | Grade |
|--------------------|--------------|
| Assignment 1 | 25% |
| Assignment 2 | 25% |
| Assignment 3 | 25% |
| Individual Project | 25% |
| Total | 100% |

Course Policies

Canvas: The course syllabus, lectures, schedule, and other relevant materials will be placed on the **Canvas (<http://canvas.vt.edu/>)** website developed for this course. Students unable to access this website should contact the instructor immediately. <https://canvas.vt.edu/>

Class Attendance: It is strongly recommended that students attend all class periods and participate in class discussions. This will be reflected in the student's grade through better performance on homework assignments and exams. However, class attendance is not formally considered in the student's final grade.

Virginia Tech Honor System: The Undergraduate Honor Code pledge that each member of the university community agrees to abide by states:

"As a Hokie, I will conduct myself with honor and integrity at all times. I will not lie, cheat, or steal, nor will I accept the actions of those who do."

Students enrolled in this course are responsible for abiding by the Honor Code. A student who has doubts about how the Honor Code applies to any assignment is responsible for obtaining specific guidance from the course instructor before submitting the assignment for evaluation. Ignorance of the rules does not exclude any member of the University community from the requirements and expectations of the Honor Code.

As a University requirement, all incidents of cheating and plagiarism must be reported by the course instructor to the VT Honor Code Panel. This includes multiple students submitting identical homework assignments. Any incidence of suspected dishonorable conduct must be reported.

For additional information about the Honor Code, click **[here \(http://www.honorsystem.vt.edu/\)](http://www.honorsystem.vt.edu/)**.

Assignments: All assignments will become available on Canvas at least one week before the due date. Assignments must be submitted electronically to Canvas by midnight of the due date. Any assignment posted (or modified) after this time will be subject to late penalty. All students must complete all assignments individually.

Late Assignments: A penalty of 10% per day will be assessed to late assignments. The time-stamp of the submission on Canvas will be used to determine if an assignment is on-time or late. Late penalties will be strictly enforced.

MATLAB: Students are expected to use the MATLAB programming language to complete assignments. A MATLAB primer is included as an Appendix in Canvas. Additional materials will be provided if necessary.

COMSOL: The COMSOL program is available through the Math Emporium. Students may have to complete tasks requiring this software on-site.











Individual Projects: One project (to be completed and submitted by each student separately) is required. Students will find an application of optimization or Finite and Spectral Element Methods in their own research projects and perform appropriate calculations. A three-page (single space) write-up is required and must contain: Introduction, Methods, Results and Discussion, Conclusions, and References sections. All MATLAB/COMSOL programs, spreadsheets, etc. must be included as Appendices.


















Make-Up Assignments: In the event that an assignment must be completed at an earlier or later date or time, written notice is required 1 week before the scheduled due date. In the case of an emergency or illness, special arrangements will be allowed as long as written documentation or a doctor's note is submitted.

















Students with Disabilities: Any student who feels he or she may need accommodation because of a disability (e.g., learning disability, attention deficit disorder, psychological, physical, etc.), please make an appointment to see me during office hours.










Principles of Community: A learning environment will be created strictly adhering to the [Virginia Tech Principles of Community](http://www.vt.edu/diversity/principles-of-community.html) (<http://www.vt.edu/diversity/principles-of-community.html>).

Assignments Summary:

| Date | Details | |
|------------------|---|--------------------|
| Mon Aug 22, 2016 |  <u>01 - Introductions and the Kyoto Encyclopedia of Genes and Genomes (KEGG) compound.txt database</u> (https://canvas.vt.edu/calendar?event_id=24490&include_contexts=course_28001) | 11:15am to 12:05pm |
| Wed Aug 24, 2016 |  <u>02 - Beginning parsing with MATLAB</u> (https://canvas.vt.edu/calendar?event_id=24491&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Aug 26, 2016 |  <u>03 - Learning to read and write text files with MATLAB</u> (https://canvas.vt.edu/calendar?event_id=24492&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Aug 29, 2016 |  <u>04 - Writing a program to parse compound.txt</u> (https://canvas.vt.edu/calendar?event_id=24493&include_contexts=course_28001) | 11:15am to 12:05pm |
| Wed Aug 31, 2016 |  <u>05 - Continuing to parse the compound.txt file</u> (https://canvas.vt.edu/calendar?event_id=24494&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Sep 2, 2016 |  <u>06 - Dealing with the NAMES of compound.txt</u> (https://canvas.vt.edu/calendar?event_id=24495&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Sep 5, 2016 |  <u>Labor Day (No Class)</u> (https://canvas.vt.edu/calendar?event_id=24496&include_contexts=course_28001) | 11:15am to 12:05pm |
| Wed Sep 7, 2016 |  <u>07 - Parsing the reaction.lst KEGG database</u> (https://canvas.vt.edu/calendar?event_id=24497&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Sep 9, 2016 |  <u>08 - A program for parsing reaction.lst</u> (https://canvas.vt.edu/calendar?event_id=24498&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Sep 12, 2016 |  <u>09 - Solving systems of coupled ordinary differential equations</u> (https://canvas.vt.edu/calendar?event_id=24499&include_contexts=course_28001) | 11:15am to 12:05pm |

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| Wed Sep 14, 2016 |  <u>10 - Writing a Runge-Kutta program in MATLAB</u> (https://canvas.vt.edu/calendar?event_id=24500&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Sep 16, 2016 |  <u>11 - Solving coupled ODEs with Runge-Kutta in MATLAB</u> (https://canvas.vt.edu/calendar?event_id=24501&include_contexts=course_28001) | 11:15am to 12:05pm |
| |  <u>Assignment 1</u> (https://canvas.vt.edu/courses/28001/assignments/78836) | due by 11:59pm |
| Mon Sep 19, 2016 |  <u>12 - Introduction to optimizing kinetic parameters</u> (https://canvas.vt.edu/calendar?event_id=24502&include_contexts=course_28001) | 11:15am to 12:05pm |
| Wed Sep 21, 2016 |  <u>13 - Kinetic parameter optimization in MATLAB</u> (https://canvas.vt.edu/calendar?event_id=24503&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Sep 23, 2016 |  <u>14 - Kinetic parameter optimization in MATLAB (continued)</u> (https://canvas.vt.edu/calendar?event_id=24504&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Sep 26, 2016 |  <u>15 - Building an optimization algorithm based on natural selection</u> (https://canvas.vt.edu/calendar?event_id=24505&include_contexts=course_28001) | 11:15am to 12:05pm |
| Wed Sep 28, 2016 |  <u>16 - Genetic algorithm operators</u> (https://canvas.vt.edu/calendar?event_id=24506&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Sep 30, 2016 |  <u>17 - Implementing the genetic algorithm</u> (https://canvas.vt.edu/calendar?event_id=24507&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Oct 3, 2016 |  <u>18 - Optimization examples</u> (https://canvas.vt.edu/calendar?event_id=24508&include_contexts=course_28001) | 11:15am to 12:05pm |
| Wed Oct 5, 2016 |  <u>19 - Concluding optimization</u> (https://canvas.vt.edu/calendar?event_id=24509&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Oct 7, 2016 |  <u>20 - Starting the finite element method in one-dimension</u> (https://canvas.vt.edu/calendar?event_id=24510&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Oct 10, 2016 |  <u>21 - The global interpolation function and the Galerkin projection</u> (https://canvas.vt.edu/calendar?event_id=24511&include_contexts=course_28001) | 11:15am to 12:05pm |
| Wed Oct 12, 2016 |  <u>22 - Formation of a linear algebraic system</u> (https://canvas.vt.edu/calendar?event_id=24512&include_contexts=course_28001) | 11:15am to 12:05pm |
| |  <u>Assignment 2</u> (https://canvas.vt.edu/courses/28001/assignments/78837) | due by 11:59pm |
| Fri Oct 14, 2016 |  <u>Fall Break (No Class)</u> (https://canvas.vt.edu/calendar?event_id=24513&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Oct 17, 2016 |  <u>No Class</u> (https://canvas.vt.edu/calendar?event_id=24514&include_contexts=course_28001) | 11:15am to 12:05pm |

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| Wed Oct 19, 2016 |  <u>23 - Formation of a linear algebraic system (part 2)</u> (https://canvas.vt.edu/calendar?event_id=24515&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Oct 21, 2016 |  <u>24 - Solving the linear algebraic system</u> (https://canvas.vt.edu/calendar?event_id=24516&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Oct 24, 2016 |  <u>25 - Solving the linear algebraic system (part 2)</u> (https://canvas.vt.edu/calendar?event_id=24517&include_contexts=course_28001) | 11:15am to 12:05pm |
| Wed Oct 26, 2016 |  <u>26 - Assembly of the linear system using MATLAB notation</u> (https://canvas.vt.edu/calendar?event_id=24518&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Oct 28, 2016 |  <u>27 - Unsteady diffusion in one-dimension</u> (https://canvas.vt.edu/calendar?event_id=24519&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Oct 31, 2016 |  <u>28 - Solving the unsteady diffusion problem in MATLAB</u> (https://canvas.vt.edu/calendar?event_id=24520&include_contexts=course_28001) | 11:15am to 12:05pm |
| Wed Nov 2, 2016 |  <u>29 - Convection in one-dimension</u> (https://canvas.vt.edu/calendar?event_id=24521&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Nov 4, 2016 |  <u>30 - One-dimensional convection-diffusion</u> (https://canvas.vt.edu/calendar?event_id=24522&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Nov 7, 2016 |  <u>31 - The finite element method in two dimensions</u> (https://canvas.vt.edu/calendar?event_id=24523&include_contexts=course_28001) | 11:15am to 12:05pm |
| Wed Nov 9, 2016 |  <u>32 - Two-dimensional interpolation and domain discretization</u> (https://canvas.vt.edu/calendar?event_id=24524&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Nov 11, 2016 |  <u>33 - Implementing the finite element method in two-dimensions with MATLAB</u> (https://canvas.vt.edu/calendar?event_id=24525&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Nov 14, 2016 |  <u>34 - Building the 2D finite element method in MATLAB</u> (https://canvas.vt.edu/calendar?event_id=24526&include_contexts=course_28001) | 11:15am to 12:05pm |
| Wed Nov 16, 2016 |  <u>35 - Introduction to COMSOL: Setup and building a geometry</u> (https://canvas.vt.edu/calendar?event_id=24527&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Nov 18, 2016 |  <u>No Class</u> (https://canvas.vt.edu/calendar?event_id=24528&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Nov 21, 2016 |  <u>Thanksgiving Break (No Class)</u> (https://canvas.vt.edu/calendar?event_id=24529&include_contexts=course_28001) | 11:15am to 12:05pm |
| Wed Nov 23, 2016 |  <u>Thanksgiving Break (No Class)</u> (https://canvas.vt.edu/calendar?event_id=24530&include_contexts=course_28001) | 11:15am to 12:05pm |

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| Fri Nov 25, 2016 |  Thanksgiving Break (No Class) (https://canvas.vt.edu/calendar?event_id=24531&include_contexts=course_28001) | 11:15am to 12:05pm |
| Mon Nov 28, 2016 |  36 - Introduction to COMSOL: Solving problems https://canvas.vt.edu/calendar?event_id=24532&include_contexts=course_28001 | 11:15am to 12:05pm |
| Wed Nov 30, 2016 |  37 - The 2D unit circle in COMSOL (https://canvas.vt.edu/calendar?event_id=24533&include_contexts=course_28001) | 11:15am to 12:05pm |
| Fri Dec 2, 2016 |  38 - Effective diffusivity in porous media in COMSOL https://canvas.vt.edu/calendar?event_id=24534&include_contexts=course_28001 | 11:15am to 12:05pm |
| Mon Dec 5, 2016 |  39 - Dealing with chemical reactions in COMSOL https://canvas.vt.edu/calendar?event_id=24535&include_contexts=course_28001 | 11:15am to 12:05pm |
| Wed Dec 7, 2016 |  40 - Reflection (https://canvas.vt.edu/calendar?event_id=24536&include_contexts=course_28001) | 11:15am to 12:05pm |
| |  Assignment 3 (https://canvas.vt.edu/courses/28001/assignments/78850) | due by 11:59pm |
| Mon Dec 12, 2016 |  Project Presentations (https://canvas.vt.edu/calendar?event_id=24826&include_contexts=course_28001) | 10:05am to 12:05pm |
| |  Project (https://canvas.vt.edu/courses/28001/assignments/78852) | due by 11:59pm |