Course 490/590 (3 Credits)

This syllabus is a sample only; please refer to the course Blackboard page for up-to-date information.

**Instructor:** Dr. Walt Loveland       lovelanw@onid.orst.edu

**Course description:** This course is intended to teach the skills necessary for using computers to aid the work of science. This course will cover data analysis and visualization, numerical methods of analysis, simulations and modeling using three programming platforms; a spreadsheet, a symbolic language and a high level programming language.

This course combines approximately 90 hours of instruction, online activities, and assignments for 3 credits.

**Prerequisites/corequisites:** One year of college chemistry is required (our examples will be drawn from general chemistry). MTH 252 is also required. No prior experience with computers is assumed, so those who are advanced users may find the early portion of the course relatively easy.

The following book is **required**, but not available from the OSU Beaver Store; you can find it on Amazon or other online resources:


**Time requirements:** You will be given 20 problems to solve during the course that are approximately linked to the 18 lessons presented in the course. You can submit each problem for evaluation multiple times until you get it correct; the instructor will comment on what is wrong when the program does not work.

**Course Content:**

- Introduction, PCs, DOS, Windows
- Spreadsheets-Basics, Tabular Calculation
- Spreadsheets, Graphs, Data I/O
- Mathematica, Introduction
- Mathematica and Data
- FORTRAN90, Introduction
- FORTRAN90, Arrays, I/O, OOP
- Statistical Characterization of Data
- Curve Fitting, Regression, Smoothing
- Simplex, NLLS
- Numerical Integration and Differentiation
- Roots of Equations
- Simultaneous Systems of Equations
- ODEs
- Fourier Analysis, Image Enhancement
- Monte Carlo Techniques
- Simulations and Models
- LaTeX

**Student Learning Outcomes:**

1. The student will demonstrate the ability to use a modern typesetting language, LaTeX, to write simple hierarchical text and to write complex equations (Problem 19).
2. The student will demonstrate the ability to use the Simplex method to do non-linear least squares fitting of data (Problem 20).
3. Students will demonstrate the ability to use Fast Fourier Transforms and Filters to filter noise from experimental data (Problem 16).
4. Students will use a fourth order Runge-Kutta method in Fortran to solve the differential equations resulting from chemical kinetics (Problem 15).
5. The student will demonstrate the ability to use a Monte Carlo method for numerical integration (Problem 6).
6. The student will demonstrate the ability to solve a multiple linear regression problem related to absorption spectroscopy (Problems 13 and 14).
7. The student will demonstrate that they can use Mathematica for root finding (problem 12).
8. The student will demonstrate the ability to use Mathematica to solve the kinetics of the catalytic decomposition of nitrous oxide and apply it to some real world data for this reaction (Problem 11).
9. The student will be able to write a working Mathematica program to calculate the fugacity of a van der Waals gas (Problem 10).
10. Student will demonstrate the ability to use a spreadsheet to solve a non-linear least squares problem (Problem 8).
11. The student will demonstrate the ability to write programs (Fortran, Spreadsheet, Mathematica) that read in a set of data and compute some elementary statistical characterizations of the data (Problems 5, 7, and 3b).
12. The student will be able to use Mathematica to solve difficult integrals and to fit data (Problem 4).
13. The student will demonstrate the ability to use the "circular reference" feature of spreadsheets to calculate the compressibility of a van der Waals gas (Problem 3a).

14. The student will demonstrate the ability to use spreadsheets to calculate the numerical solutions to common problems in the physical sciences (Problems 1 and 2).

**Exams:** Grading of this course is based on the problems assigned; there are no exams. Students are expected to do the problems without collaboration.

**Grading (CH 490):**

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**Grading (CH 590):**

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**Services for Students with Disabilities:**

Accommodations are a collaborative effort between students, faculty, and the Disability Access Services (DAS) office. Students with accommodations approved through DAS are responsible for contacting the faculty member in charge of the course prior to, or during, the first week of the term to discuss accommodations. Students who believe they are eligible for accommodations, but who have not yet obtained approval through DAS, should contact DAS immediately at 541-737-4098.

**Expectations for Student Conduct:**

Student conduct is governed by the universities policies, as explained in the Office of Student Conduct: Information and Regulations. In an academic community, students and faculty, and staff each have responsibility for maintaining an appropriate learning environment, whether online or in the classroom. Students, faculty, and staff have the responsibility to treat each other with understanding, dignity, and respect. Further information may be found at: http://oregonstate.edu/studentconduct/
Academic Integrity:

Students are expected to comply with all regulations pertaining to academic dishonesty, defined as: *An intentional act of deception in which the student seeks to claim credit for the work or effort of another person or uses unauthorized materials or fabricated information in any academic work.* For further information, visit Avoiding Academic Dishonesty, or contact the office of Student Conduct and Mediation at 541-737-3656.

Conduct in this online classroom:

Students are expected to conduct themselves in the course (e.g. on discussion boards, email postings) in compliance with the university's regulations regarding civility. Students will be expected to treat all others with the same respect as they would want afforded to themselves. Disrespectful behavior (such as harassing behavior, personal insults, inappropriate language) or disruptive behaviors are unacceptable and can result in sanctions as defined by Oregon Administrative Rules Division 015 Student Conduct Regulations.

Student Evaluation of Teaching:

We encourage you to engage in the course evaluation process each term – online, of course. The evaluation form will be available toward the end of each term, and you will be sent instructions through ONID. You will login to “Student Online Services” to respond to the online questionnaire. The results on the form are anonymous and are not tabulated until after grades are posted.

NOTE to prospective students: This syllabus is intended to provide students who are considering taking this course an idea of what they will be learning. A more detailed syllabus will be available on the course Blackboard site for enrolled students and may be more current than this sample syllabus.