



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 Canvas site for enrolled students and may be more current than this sample syllabus.

**CH 490/590
COMPUTER PROGRAMMING FOR SCIENTISTS**

Credits: 3

Instructor

LOVELAND
lovelanw@onid.orst.edu
541-737-7078

Course Description

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. The high level language will be chosen by each student from a list of three possibilities

Prerequisites

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

Communication

How will we keep in touch?

Currently the primary way with which you will be given assignments and material will be having it posted on this webpage. The current way for you to communicate with your instructor is through email (lovelanw@onid.orst.edu). Please use your onid email address for such communications. We will not be able to deal with email from non-onid addresses.

The instructor will reply to course-related questions and email within 24-48 hours. He will strive to return your assignments and grades for course activities to you within five days.

Course Credits

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

Technical Assistance

If you experience computer difficulties, need help downloading a browser or plug-in, assistance logging into the course, or if you experience any errors or problems while in your online course, contact the OSU Help Desk for assistance. You can call (541) 737-3474, email osuhelpdesk@oregonstate.edu or visit the [OSU Computer Helpdesk](#) online.

Learning Resources

Textbooks

Two textbooks are required of all students. They are: Billo, Excel for Chemists, 3rd Edition and Ruskeepaa, Mathematica Navigator, 3rd Edition. These books may be purchased at Amazon. The OSU Store does not carry these books.

A third textbook should be chosen by the student and purchased accordingly. Students are given a choice of which high level language they can choose to use in solving problems. The choices are FORTRAN, PYTHON or C++. The recommended textbooks are: FORTRAN (Nyhoff and Leestma, FORTRAN 90 for Engineers and Scientists), C++ (Nyhoff, Programming in C++ for Engineering and Science) and PYTHON (Langtangen, A Primer on Scientific Programming with Python)

You will also need access to computers with the following capabilities:

- Internet Access (including a web browser and email capability)
- A version of Microsoft Excel (the more up-to-date, the better). The student version of Excel sells for about \$80 but Excel is also included in the Office package present on many computers.
- A copy of Mathematica (the current version is 10.0). The student version of Mathematica currently sells for \$140. A six month access version of Mathematica can be downloaded for \$70 at <http://store.wolfram.com/view/app/timedstudent/semester.str>
 - When you choose the high level language, you will be given directions on how to download appropriate software.

Note to prospective students: Please check with the OSU Bookstore for up-to-date information for the term you enroll ([OSU Bookstore Website](#) or 800-595-0357). If you purchase course materials from other sources, be very careful to obtain the correct ISBN.

Canvas

This course will be delivered via Canvas where you will interact with your classmates and with your instructor. Within the course Canvas site you will access the learning materials, such as the syllabus, class discussions, assignments, projects, and quizzes. To preview how an online course works, visit the [Ecampus Course Demo](#). For technical assistance, please visit [Ecampus Technical Help](#).

Measurable Student Learning Outcomes

What topics will be discussed? Here is the tentative list of topics to be discussed, in approximate order of introduction:

- Topic:
- 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
- What are the student learning outcomes for this course?
- Student Learning Outcomes and their Relation to the Assigned Problems.
- 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 (Problem 13,14)
- 7. The student will demonstrate that they can use Mathematica for root finding (problem 12).
- 8. The student will demonstrate the ability to do numerical simulations (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,

Mathematica) that read in a set of data and compute some elementary statistical characterizations of the data (Problems 5,7)

- 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).

Evaluation of Student Performance

What are the class requirements, and how is this course graded? 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 and we will comment on what is wrong when the program does not work. The last day for receipt of problems is 1700 17 MARCH, 2017. Please email all problem solutions to lovelanw@onid.orst.edu as attachments to the email. Problems will be graded P or N based strictly on whether you get the correct answer.

No partial credit is given. The programs must give the correct answer. Course grades for Ch 490 will be determined as follows:

- Number of Problems correct • Grade
- 13 = • A
- 11 = • B
- 9 = • C
- 8 = • D
- These problems are the equivalent of the usual examinations. For students taking Ch 590, the same table applies but two more problems are needed for a given grade. Thus, for an A grade in Ch490, you need 13 correct problems while for an A grade in Ch 590 you need 15 problems, etc. Only letter grades are given, no + or --- grades. No I grades are given.

Because no tests, etc. are given, these problems take the place of the traditional tests. Therefore the work on each problem must be independent work, just as though you were taking a test. **Collaboration is strictly forbidden.**

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Course Policies

Warning: Because of the large number of students enrolled in Chemistry web classes, the ability to offer help, etc. during the last two weeks of the term is severely limited. We will do our best to answer all inquiries about content within 7 business days but this is frequently not possible during the last two weeks of the term. Please plan ahead and submit your work as soon as possible. MULTIPLE GRADING OF PROBLEMS DURING THE LAST TWO WEEKS OF THE TERM IS NOT POSSIBLE.

This course is offered through Oregon State University Extended Campus. For more information, contact:
Web: ecampus.oregonstate.edu Email: ecampus@oregonstate.edu Tel: 800-667-1465

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- PROCRASTINATION: MANY STUDENTS GET "A" GRADES IN THIS COURSE. SOME GET "F" GRADES. THE DIFFERENCE IS THAT THE "A" STUDENTS SOLVE 1---3 PROBLEMS PER WEEK STARTING WITH WEEK 1 WHILE THE "F" STUDENTS START WORK IN THE 7TH WEEK OR LATER.

Guidelines for a Productive and Effective Online Classroom

Students are expected to conduct themselves in the course (e.g., on discussion boards, email) in compliance with the university's regulations regarding civility.

Civility is an essential ingredient for academic discourse. All communications for this course should be conducted constructively, civilly, and respectfully. Differences in beliefs, opinions, and approaches are to be expected. In all you say and do for this course, be professional. Please bring any communications you believe to be in violation of this class policy to the attention of your instructor.

Active interaction with peers and your instructor is essential to success in this online course, paying particular attention to the following:

- Unless indicated otherwise, please complete the readings and view other instructional materials for each week before participating in the discussion board.
- Read your posts carefully before submitting them.
- Be respectful of others and their opinions, valuing diversity in backgrounds, abilities, and experiences.
- Challenging the ideas held by others is an integral aspect of critical thinking and the academic process. Please word your responses carefully, and recognize that others are expected to challenge your ideas. A positive atmosphere of healthy debate is encouraged.

Statement Regarding Students with Disabilities

Accommodations for students with disabilities are determined and approved by Disability Access Services (DAS). If you, as a student, believe you are eligible for accommodations but have not obtained approval please contact DAS immediately at 541-737-4098 or at <http://ds.oregonstate.edu>. DAS notifies students and faculty members of approved academic accommodations and coordinates implementation of those accommodations. While not required, students and faculty members are encouraged to discuss details of the implementation of individual accommodations.

Accessibility of Course Materials

All materials used in this course are. If you require accommodations please contact [Disability Access Services \(DAS\)](#).

Additionally, Canvas, the learning management system through which this course is offered, provides a [vendor statement](#) certifying how the platform is accessible to students with disabilities.

Expectations for Student Conduct

Student conduct is governed by the university's policies, as explained in the [Student Conduct Code](#).

Academic Integrity

Students are expected to comply with all regulations pertaining to academic honesty. For further information, visit [Student Conduct and Community Standards](#), or contact the office of Student Conduct and Mediation at 541-737-3656.

OAR 576-015-0020 (2) Academic or Scholarly Dishonesty:

- a) Academic or Scholarly Dishonesty is defined as an act of deception in which a Student seeks to claim credit for the work or effort of another person, or uses unauthorized materials or fabricated information in any academic work or research, either through the Student's own efforts or the efforts of another.
- b) It includes:
 - i) CHEATING - use or attempted use of unauthorized materials, information or study aids, or an act of deceit by which a Student attempts to misrepresent mastery of academic effort or information. This includes but is not limited to unauthorized copying or collaboration on a test or assignment, using prohibited materials and texts, any misuse of an electronic device, or using any deceptive means to gain academic credit.
 - ii) FABRICATION - falsification or invention of any information including but not limited to falsifying research, inventing or exaggerating data, or listing incorrect or fictitious references.
 - iii) ASSISTING - helping another commit an act of academic dishonesty. This includes but is not limited to paying or bribing someone to acquire a test or assignment, changing someone's grades or academic records, taking a test/doing an assignment for someone else by any means, including misuse of an electronic device. It is a violation of Oregon state law to create and offer to sell part or all of an educational assignment to another person (ORS 165.114).
 - iv) TAMPERING - altering or interfering with evaluation instruments or documents.
 - v) PLAGIARISM - representing the words or ideas of another person or presenting someone else's words, ideas, artistry or data as one's own, or using one's own previously submitted work. Plagiarism includes but is not limited to copying another person's work (including unpublished material) without appropriate referencing, presenting someone else's opinions and theories as one's own, or working jointly on a project and then submitting it as one's own.
- c) Academic Dishonesty cases are handled initially by the academic units, following the process outlined in the University's Academic Dishonesty Report Form, and will also be referred to SCCS for action under these rules.

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](#).

OSU Student Evaluation of Teaching

Course evaluation results are extremely important and are used to help me improve this course and the learning experience of future students. Results from the 19 multiple choice questions are tabulated anonymously and go directly to instructors and department heads. Student comments on the open-ended questions are compiled and confidentially forwarded to each instructor, per OSU procedures. The online Student Evaluation of Teaching form will be available toward the end of each term, and you will be sent instructions via ONID by the Office of Academic Programs, Assessment, and Accreditation. You will log in 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.