Chemistry and the Computer

CHEM 101 – CHEMISTRY AND THE COMPUTER Fall 2014
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Office: DH-004, 924-4970  Lecture: DH 503

Class Meetings / Office Hours:

Lecture:  T and Th  10:30-11:20 a.m.  DH-503
Activity: T and Th  11:30-12:20 p.m.  DH-503
Office Hours: T and Th 09:30 – 10:20 or by appointment  DH-004

Prerequisites:  Chem 55, Math 030 or 030P with grades of "C" or better; "C-" not accepted.

Text: None required. Useful resources include “Excel for Chemists” and “Numerical Recipes for Chemists”

Lecture Notes and Activity Instructions: These will be distributed via the course website on Canvas. https://sjsu.instructure.com/

Objectives: Demonstrate competence in the use of Microsoft Excel for the archiving, analysis and tabular and visual presentation of scientific data. Demonstrate competence in solving chemical problems using Excel, Excel Visual Basic for Applications (VBA). Demonstrate ability to use molecular mechanics and quantum chemical software tool WebMO to calculate energy and molecular properties. Time permitting; we will examine some available tools for managing citations when writing technical papers.

The above objectives fall within objectives 1-5, 8 and 10 the Chemistry Department Program Learning Objectives for the BS and BA in Chemistry.

Tentative Grading Structure: A single letter grade will be assigned for Chem 101. The final exam will be on Tuesday, December 16 from 945-1200.

Lecture Grade: 50% of the total grade, based on exams and quizzes. Material on the exams will be based on the lecture and homework assignments.

Activity Grade: 50% of the total grade. This will be based on assignments mainly done during the activity session.

Preliminary plans for grading structure:

Lecture Grade: 300 points
Midterm exam: 100 points
Final two-hour exam: 100 points
6 Quizzes: 100 points

Activity Grade: 300 points
15 Exercise assignments: 300 points

Approximate Total: 600 points

Grading scale by percent of total points:

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San José State University
<table>
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<th>Week</th>
<th>Overview of Proposed Lecture Topics</th>
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| 1    | **Basics of Computers and MS Office:** Excel, and Word  
      | Processors, operations, stack, cache, storage, basic  
      | operations, file systems, file formats, numeric formats  
      | (binary, bcd, floating point). Data types in  
      | programming: Boolean, integer, float, string, etc.  
      | Representation of integers, signed integers and real  
      | numbers. ASCII text convention. |
| 1    | **Display of Quantitative Information I** Textual  
      | Number formatting, significant figures and symbols.  
      | Table formatting. Display of units. "Paste special to  
      | preserve data." Audit trails: file names, paths, dates  
      | and conditions. Information management. Equation  
      | editor. |
| 1    | **Display of Quantitative Information II** Visual  
      | Data import and export, graphing to scientific  
      | standards, scaling, formatting, dealing with different  
      | number formats. Use of text editor (Notepad), Binary  
      | editors and Excel. |
| 2    | **Basic Chemical Calculations**  
      | Chemical functions: plots to extract information:  
      | Gas Laws, solubility, pH and complexation. |
| 3    | **Programming in VBA**  
      | Syntax, basic concepts and interfacing with Excel  
      | worksheets. Making and using user-defined functions. |
| 4    | **Generalized Multivariate Least Squares Regression**  
      | Theory and application of univariate and multivariate  
      | least squares analysis using in-spreadsheet matrix  
      | manipulation, Visual Basic and analysis tools "Linest"  
      | and "Regression" |
| 5    | **Statistical Calculations**  
      | Excel exercises in statistics: Descriptive aspects  
      | mean, median, mode, standard deviation, confidence  
      | tests. Data Modeling by Regression |
| 6    | **Propagation of Random Uncertainty: Simulation and Theory**  
      | Discrete distributions generated by variable input  
      | variables. Differential error propagation methods. |
| 7    | **Monte-Carlo Methods**  
      | Error propagation by extrema and by random number  
      | generation. Calibration curve examples. |
| 8    | **Calibration Methods**  
      | Using Excel to deal with external and internal  
      | standards, standard additions, spike recovery and  
      | quality control standards. |
| 8    | **Iteration and Data Import**  
      | Further VBA concepts, Macro recording and  
      | adaptation. |
| 9    | **Advanced Equilibria**  
      | Exact solutions by computational approximation.  
      | Minimization using successive convergent  
      | approximation and via the golden mean method. |
| 10   | **Spectral Fitting**  
      | Multivariate Linear and Non-linear regression |
| 11   | **Titration Curves: Modeling and fitting**  
      | Single and multiple equilibrium modeling of titration  
      | data: pH versus volume of titrant, pCa, pCl etc. |
| 12   | **Smoothing Methods**  
      | Smoothing functions, moving average, triangular,  
      | Gaussian. |
| 12   | **Discrete Fourier Analysis**  
      | Basic concepts and theorems, issues attending  
      | discrete signal processing (Nyquist theorem, aliasing  
      | etc.) signal recovery, smoothing. |
| 13   | **Diffusion Simulation**  
      | Simulation of boundary condition problems. |
| 14   | **Cross correlation and Autocorrelation analysis**  
      | Fourier and discrete correlation analysis for signal  
      | recovery. Examples from flow cytometry and dynamic  
      | light scattering. |
| 15   | **Molecular Mechanics / Quantum Calculations**  
      | Introduction to the WebMO interface to Firefly  
      | molecular modeling and calculation software.  
      | Structural determination, normal modes of vibration  
      | and UV spectral prediction. |

Time permitting we may also have instruction in the following:

| Data Acquisition | Analog to digital conversion (ADC) and digital to  
                  | analog (DAC), bit depth, conversion speed, conversion  
                  | methods. |
| Refworks         | Bibliographic software |
| Search tools     | Google Scholar, Web of Science, Science Direct |
Due Dates and Policy on Late Work
I plan to have all material submitted via D2L, so submission after the due date will not be possible except in extenuating circumstances and by agreement with me. Exercises will typically be due at the end of the activity period.

Drop Policy:
The deadline to drop classes without a W is Tuesday, September 6th. The deadline to add is Tuesday, September 13th. After the regular drop period ends, only documented medical or similar emergencies will be accepted as a valid reason to drop a course. Note particularly that a change in work schedule is no longer an acceptable reason. Therefore, it is critical that you inform your employer that you have a serious commitment for your scheduled class and laboratory times during the whole semester. If your employer cannot guarantee that you can meet this obligation, then you should drop the class in order to allow someone who can fulfill this commitment to register. Also, be aware of the fact that “unsatisfactory performance in course work and protection of your GPA is not a serious and compelling reason in itself for requesting permission to drop”. After the twentieth day of instruction, all petitions to drop classes or withdraw from school will be reviewed by the Director of Academic Services. Petitions are available in the Student Resource Center.

ADDENDUM TO ALL CHEMISTRY DEPARTMENT GREENSHEETS
(Except Chem 291 Sections)
Revised August 2002

CHEMICAL SAFETY – all courses

Chem 120S is a required course for all chemistry majors and minors and a prerequisite for all Chem 180/298 research.

EMERGENCIES AND EVACUATIONS – all courses

If you hear a continuously sounding alarm, or are told to evacuate by Emergency Coordinators (colored badge identification), walk quickly to the nearest stairway (end of each hall). Take your personal belongings, as you may not be allowed to immediately return. Follow instructions of Emergency Coordinators. Be quiet so you can hear. Once outside, move away from the building. Do no return to the building unless the Police or Emergency Coordinators announce that you may.

DISABLED STUDENTS – all courses

Campus policy in compliance with the Americans with Disabilities Act: "If you need course adaptations or accommodations because of a disability, or if you need special arrangements in case the building must be evacuated, please make an appointment with me as soon as possible, or see me during office hours. Presidential Directive 97-03 requires that students with disabilities requesting accommodations must register with DRC to establish a record of their disability."
ACADEMIC INTEGRITY STATEMENT – all courses (from the Office of Student Conduct and Ethical Development):

"Your own commitment to learning, as evidenced by your enrollment at San José State University, and the University's Academic Integrity Policy requires you to be honest in all your academic course work. Faculty members are required to report all infractions to the Office of Student Conduct and Ethical Development. The policy on academic integrity can be found at http://sa.sjsu.edu/student_conduct.

LABORATORY SAFETY – all laboratory courses

You should read the safety section of the SJSU Catalog under Chemistry Department (page 121 in the 2006/08 Catalog). Note in particular: "Failure to comply with proper procedures and prescribed safety cautions shall subject the student to disciplinary action. 1) Any student who engages in unauthorized experimentation, or who seriously disregards safety, thereby endangering self or others shall be withdrawn immediately from the class with a grade of F. 2) Any student who shows persistent disregard for safety may have his/her grade lowered, and may risk being withdrawn with a final grade of F."

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