Course Syllabus

Outline: COMS 7100 is an intense hands-on course in computational methods as applied to solving problems in various disciplines of Natural Sciences. Possible topics include computational aspects of linear algebra and contemporary numerical methods.

Prerequisites: Undergraduate Calculus and Differential Equations courses, and the following PhD-level courses: Fundamentals of Computational Science (COMS 6100), Fundamentals of Scientific Computing (COMS 6500), and possibly Data Abstraction and Programming Fundamentals (CSCI 6020). A solid background in computer-algebra environments such as Matlab, Maple, Scilab or Mathematica etc. is required. Expertise in a computer language such Fortran, C/C++ etc. is highly recommended.

Instructor: Dr. Anatoliy Volkov ("Dr. V"), Associate Professor of Chemistry
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E-mail: Anatoliy.Volkov@mtsu.edu
Office hours via Zoom: M: 10:0 am – 2:00 pm W: 10:00 am – 2:00 pm
Other times – by appointment only
To sign up for a Zoom meeting, use http://calendly.com/avolkov/office-hours-via-zoom

Meetings: T, R 9:40 am – 11:30 am; Business and Aerospace Bldg (BAS) S343
Final Exam date: Thursday, May 6 10:00 am – noon; Business and Aerospace Bldg (BAS) S343

Textbook: None required. A detailed handout for each topic is available on D2L. A list of helpful auxiliary textbooks includes, but is certainly not limited to:

Press, W. H., Teukolsky, S. A., Vetterling, W. T., Flannery, B. P. *Numerical Recipes 3rd Edition: The Art of Scientific Computing*, 3rd edition. Cambridge University Press, 2007.

Tam, P. T. *A Physicist's Guide to Mathematica, Second Edition*. Academic Press, 2008.

Arfken, G. B., Weber, H. J., Harris, F. E. *Mathematical Methods for Physicists, Sixth Edition*. Academic Press, 2005.

Stoer, J. & Bulirsch, R. *Introduction to Numerical Analysis (Texts in Applied Mathematics, Book 12)*. Springer, 2002.

Guide to Available Mathematical Software http://gams.nist.gov/

Netlib - a collection of mathematical software, papers, and databases. http://www.netlib.org/

Numerical Recipes Software http://numerical.recipes/

Class format: Each meeting will consist of a short lecture (if necessary) and a hands-on computational project that will also be your homework. There is no textbook assigned for the course. Each topic/project will be accompanied by a handout available for download from D2L. You absolutely need to read handouts before coming to class or else you will be wasting your own [presumably, valuable] time! If you need my help debugging your code, you should bring your own laptop to *each* meeting, including the *first* meeting on **January 26**, with your choice of computational environment installed (Mathematica, Matlab, Maple, Scilab, C/C++/Fortran etc.). Please have the second programming environment (for example, Mathematica) installed by **February 9**. FYI, if you are an MTSU employee (for example, a TA), you can get a free copy of Mathematica (Mac, Windows, Linux) for any number of your own computers. It is called "Mathematica at Home", see http://www.mtsu.edu/itd-client-services/site-license.php#Wolfram. To apply for Mathematica-at-Home license, submit a request at http://www.wolfram.com/siteinfo/homeuse/?parent_license=L3095-6651&request_type=NEW_HU_LICENSE. Alternatively, you can always connect to the CS Dept. server "shemp" or use the MTSU Citrix Workspace environment that has Mathematica, Maple, and Matlab installed. For each project, a completed working code must be uploaded to an appropriate D2L dropbox by the assigned due date/time. Submissions by email will not be accepted!

WARNING !!! While you are allowed (and even encouraged!) to discuss the project material and implementation with your classmates, YOU ARE ABSOLUTELY **NOT** ALLOWED TO COPY EACH OTHER'S CODE!

Grading: In addition to submitting a completed project on D2L, each student must present his/her project in front of the entire class. A presentation should be given in a clear voice, loud enough to be heard everywhere in the classroom. Each project shall be graded on a scale from 0 to 100. Missing a presentation will incur an automatic deduction of **30%**. A detailed description of the grading criteria is given in a Table below. The grading of each project starts at 100%. Even if one criterion for a score of 100% is not satisfied, the grading continues using the 90.0 – 99.9% criteria. Even if one criterion for that score is not satisfied, the grading continues using the 80.0 – 89.9% criteria, and so on…

Project Score (%)	Justification
100	*All objectives* as described in the handout under "Computational exercise. Objectives" *are achieved*. It means that **1)** the code gives correct results for all input files provided (input files must not be modified!), **2)** the printout is as described in the objectives, **3)** the execution time is below the time limit given in the objectives (if any) or 1 hour per input file (whichever is greater), **4)** the code was submitted to D2L by the due date/time.
90.0 – 99.9	*Most of the objectives* as described in the handout under "Computational exercise. Objectives" *are achieved*. It means that **1)** the code gives *mostly* correct results for all input files provided (input files must not be modified!), **2)** the printout is *mostly* as described in the objectives, **3)** the execution time is below the time limit given in the objectives (if any) or 1 hour per input file (whichever is greater), **4)** the code was submitted to D2L by the due date/time. Points may have been deducted for miscellaneous (not significant) issues with results and printout due to simple typos, but nothing serious (i.e. no fundamental errors).
80.00 – 89.9	The code gives correct results for most of the input files (input files must not be modified!), but fails for some due to *few* incorrect mathematics, programming, and science statements. The printout may only roughly follow the guidelines. The execution time is within or slightly above (not more than 10%) the time limit described in the objectives (if any) or 1 hour per input file (whichever is greater). The code was submitted to D2L by the due date/time.
70.0 – 79.9	The code was submitted to D2L late (as judged by the D2L filestamp) but within 24 hours of the established deadline. Input files need to be modified to make the code run. There may be *some* significant issues in the code related to mathematics, science, and programming, which make the code often produce incorrect results. The execution time may be 11% - 30% above the time limit described in the objectives (if any) or 1 hour per input file (whichever is greater). There may be significant issues with the printout. For example, very limited printout (i.e. much less than what is requested in the objectives).
50.0 – 69.9	The code may have *many* significant issues errors in mathematics, science, or programming, which makes the code produce mostly incorrect results. The code was submitted to D2L late (as judged by the D2L filestamp) but within 25 – 96 hours of the established deadline. The execution time may be 31 – 50% above the time limit described in the objectives (if any) or 1 hour per input file (whichever is greater). No printout.
00.0 – 49.9	The code was never submitted to D2L, or submitted more than 96 hours after the established deadline (as judged by the D2L filestamp). The code may have *too many* fundamental flaws in mathematics, science, and programming. The code pretty much always gives incorrect results. The execution time is more than 50% above the time limit described in the objectives (if any) or 1 hour per input file (whichever is greater).

Language of instruction. **The official language of instruction is English.** All teaching, exercise and practical material are provided in English. Please refrain from using a foreign language in the classroom.

Course Requirements: In order to promptly complete the objectives of the course you are required to:

a. Read and study project assignments.
b. Attend class meetings.
c. Participate in class activities.
d. Solve assigned problems.
e. Turn in completed projects on time.

Homework: Your homework includes completion of the assigned project and researching the next topic (see the class schedule and handouts posted to D2L).

D2L submission notes:

- ALL files submitted to D2L must be UNARCHIVED and UNCOMPRESSED. Submitting compressed and/or archived files to D2L will result in additional [if applicable] automatic deduction of **30%**.
- You MUST also provide instructions on how to [if necessary] compile and run your code, and include ALL auxiliary files [if used]. Failure to do so will result in additional [if applicable] automatic deduction of **30%**.
- If several revisions of the same document are submitted to D2L, only the latest revision will be graded, unless a note is provided on D2L specifying which revision needs to be graded.
- **ALL LATE SUBMISSIONS ARE SUBJECT TO AN AUTOMATIC DEDUCTION OF 50% !!!**

Study Guide: There is no study guide for this course. Please, do not ask for one!

Extra credit: No opportunities for extra credit will be available. Please, do not ask!

Final grades: The total course score will be calculated as the average of *all* assigned projects. Letter grades will be assigned according to the following scale:

90.0 - 100% = **A**
80.0 - 89.9% = **B**
70.0 - 79.9% = **C**
50.0 - 69.9% = **D**
00.0 - 49.9 % = **F**

A grade of **I** will be given only in compliance with the university policy.

E-mail correspondence: When you use commercial e-mail accounts for communicating with faculty there is a possibility of your messages being detected as spam and not delivered. To avoid this kind of issues it is recommended that you use your official MTSU e-mail account when corresponding with me. For more information, see the "*18 Etiquette Tips for E-mailing Your Professor*" handout available on D2L.
Note 1: Always include your first and your last name in your message.
Note 2: Please do NOT use D2L to communicate with me.

Students with disabilities: If you have a disability that might require assistance or accommodation, please notify me as soon as possible. You may also contact the Disability & Access Center (KUC 107; 898-2783; dacemail@mtsu.edu) with questions about such services.

Important dates:

The last day to drop or withdraw WITHOUT a grade is **February 7.**
The last day to drop or withdraw with a grade of "W" is **March 31.**
The last day to withdraw from the University (drop all classes) and receive a grade of "W" or "F" as determined by the instructor is **April 28.**

Note: You should be aware that dropping or withdrawing from this class may adversely affect scholarships or loans. In some cases, you may be required to pay back money that you received. You should check with the financial aid office before withdrawing from or dropping any class.

Academic integrity:

Plagiarism, cheating, and other forms of academic dishonesty are prohibited. According to Policy 312, Academic Misconduct,
http://www.mtsu.edu/policies/academic-affairs-students/312.php
plagiarism, cheating, and fabrication are defined as follows:

(1) Plagiarism. The adoption or reproduction of ideas, words, statements, images, or works of another person as one's own without proper attribution. This includes self-plagiarism, which occurs when an author submits material or research from a previous academic exercise to satisfy the requirements of another exercise and uses it without proper citation of its reuse.
(2) Cheating. Using or attempting to use unauthorized materials, information, or aids in any academic exercise or test/examination. Cheating includes unapproved collaboration, which occurs when a student works with others on an individual academic exercise without the express permission of the faculty member.
(3) Fabrication. Unauthorized falsification or invention of any information or citation in an academic exercise.

Anyone cheating on a project, will not only get zero for that project, but will have his/her final class score automatically reduced by **50%.** Violations of academic integrity will be sanctioned pursuant to the "MTSU Student Handbook".

Academic freedom:

According to Policy 201, Academic Freedom and Responsibility,
http://www.mtsu.edu/policies/academic-affairs-institution-and-faculty/201.php
"*Faculty members are entitled to freedom in the classroom in discussing their subject, being careful to avoid the persistent intrusion of matter, controversial or not, that has no bearing on the subject of instruction. Controversial material that pertains to the subject of instruction, even if it is likely to offend some people, is protected by this policy.* "

In my class, I teach well established scientific concepts in the field of Applied Computational Science. I do **not** discuss topics that are not related to the subject of Applied Computational Science.

That said, I reserve the right to use teaching methods in my class that I believe are most effective.

Behavior in class:

Please do not disturb the class by habitually walking in late If you get to class later (>15 minutes) you may be refused entry. Sleeping in class and other flagrant exhibitions of inattention (computer and/or phone usage etc.) will not be tolerated. Cell phones' ringing in class is highly disruptive and will not be tolerated. In addition, text messaging, any form of electronic communication, use of iPods and other multimedia devices while class is underway is not allowed (see the "College of Basic and Applied Sciences Policy for Appropriate Use of Hand-held and Wireless Technology" section of this syllabus). Also, please do not bring food to class!

Anyone disturbing class will be warned once; the second time will mean expulsion.

Use of electronic communication or wireless devices during quizzes, examinations, or other graded activities is considered as a form of cheating, and will immediately warrant disciplinary action under the terms of the Code of Student Conduct. If you use any electronic communication or wireless devices during a quiz/test/exam, you will automatically get a score of zero for that quiz/test/exam, and will be referred to the Provost Office for disciplinary action.

Note that inappropriate classroom activities, such as (but not limited to):

a) late arrivals or early departures without permission,
b) overt inattentiveness (sleeping in class, reading materials that are not related to the subject of discussion, or doing other homework in class),
c) inappropriate communication while class is in session (speaking while the instructor is speaking),
d) use of electronic communication or wireless devices, etc.

are classified as "disciplinary offenses" and may be considered as "[a]cademic and [c]lassroom [m]isconduct".

I will exercise my right to "*order the temporary removal or exclusion from the classroom of any student engaged in disruptive conduct or conduct that violates the general rules and regulations of the institution for each class session during which the conduct occurs*."

It means, for example, that if a student is more than 15 minutes late, the student will be refused entry. If the student does not comply, I will call the MTSU Police Department, and police officers will escort the student from the classroom. I will also report the student to the Office of Student Conduct for "*[f]ailure to comply with directions or directives of Institutional officials acting in the performance of their duties*", section III.B.2, "Failure to Cooperate with Institutional Officials", Policy 540, Student Disciplinary Rules,

http://www.mtsu.edu/policies/student-affairs/540.php

Note that the late arrival rule is clearly outlined in this syllabus, and failure to comply will have a negative impact on your academic career.

Table 1. Tentative class schedule. **The schedule is subject to change!**

Meeting #	Date	Projects	Project Due Date*
1 2 3 4	1/26 1/28 2/2 2/4	**Project 1 (software of your choice)**. Non-Linear Least Squares in Chemical Thermodynamics. Minimization methods: steepest descent, Gauss-Newton, Levenberg-Marquardt.	**February 9** 9:30 am
5	**2/9**	Presentations of the **Project 1** codes. Start **Project 1a**.	
6 7	2/11 2/16	**Project 1a**. Same as Project 1 but coded in a different software than that used for Project 1	**February 18** 9:30 am
8	**2/18**	Presentations of the **Project 1a** codes. Start **Project 2**.	
9 10 11 12	2/23 2/25 3/2 3/4	**Project 2 (software of your choice).** Computational Crystallography. Fourier series, Fourier transforms, Optimization methods: Newton-Raphson and eigenvector following	**March 9** 9:30 am
13	**3/9**	Presentations of the **Project 2** codes. Start **Project 3.**	
14 15 16	3/11 3/16 3/18	**Project 3 (software of your choice).** Planetary motion. Equation of motion in Classical Physics: Newton, Lagrange, and Hamilton formulations. Numerical solution of equation of motion of planets in the Solar System in 2D and 3D - Euler and midpoint methods (RK2).	**March 23** 9:30 am
17	**3/23**	Presentations of the **Project 3** codes. Start **Project 4.**	
18 19 20 21 22	3/25 3/30 4/1 4/6 4/8	**Project 4 (software of your choice).** Intro to Quantum Mechanics: operators, Schrödinger equation, separation of variables, hydrogen atom wavefunctions, Laguerre and Legendre polynomials, spherical harmonics, analytical integration in 1D, 2D and 3D	**April 13** 9:30 am
23	**4/13**	Presentations of the **Project 4** codes. Start **Project 5.**	
24 25 26	4/15 4/20 4/22	**Project 5 (software of your choice).** Variational solution of the Schrödinger equation for a hydrogen atom	**April 27** 9:30 am
27	**4/27**	Presentations of the **Project 5** codes.	
		Corrections to any one of the projects	**May 6** 9:50 am
28	**5/6**	Presentations of the **corrected** codes (class starts at 10:00 am)	

* Must be submitted to D2L dropbox by the date/time indicated.

WARNING! ALL LATE SUBMISSIONS ARE SUBJECT TO A 50% DEDUCTION!

Observed Holidays - no classes

3/12 – Study Day