Computer Science 3731/6906

Introduction to Scientific Computing/Numerical Methods (Section 001) Fall 2020



Department of Computer Science

Instructor: George Miminis

Virtual Office Hours: during allotted class time – Tues and Thurs 09:00-10:15am

E-mail: george@mun.ca (***please use this email to contact me, not D2L***)

Note that I **DO NOT** check email in Brightspace (D2L). Please send any emails to my **george@mun.ca** address, rather than my D2L address. Also, please include **[COMP3731/6906]** in the subject line. Official email correspondence within the university must be via a valid **@mun.ca** email account.

Course Content: https://online.mun.ca/

Credit Restriction:

Mathematics 3132

Prerequisites:

COMP 1001 or the former COMP 2710, Mathematics 2000, Mathematics 2050

Course Objectives:

The development of efficient algorithms for the numerical solution of some generic mathematical problems and their implementation on conventional computers, is the objective of this course. The efficiency of these algorithms with respect to **speed** (computation and data communication), **storage requirements**, but more importantly **accuracy** (due to **floating point arithmetic**), will be considered. With respect to the latter, the **numerical stability** of some **algorithms**, as well as the sensitivity of selected **problems** to **perturbations** in the **data** will be studied.

Textbook:

- There is no official textbook. My course notes will be adequate.
- However, if you would like to consult a textbook, the book by **Dahlquist & Bjorck** (in the references, later in this document) is, in my view, one of the best in the literature, but it is not for the faint-hearted.
- A list of other quite useful books can be found in the references. It is important to know that most books published by *SIAM* and *Springer* are available to MUN students free of charge, through QEII library.

Evaluation:

The final grade in this course will be determined as follows:

Assignments 30% Midterm examination 30%

(Thursday, October 22, 2020, 9:00am-10:15am Newfoundland Time)

Final examination 40%

(during regular exam period Dec 9 – 18)

Lecturing Format:

Folks, we are sailing uncharted waters, and although a lot of thought has been put in the organization of novel, online teaching styles, changes may need to be made on the fly. So please be up-to-date with possible course announcements posted on the course's **Brightspace (D2L)** shell. Once an announcement has been made, it will be assumed that it has been absorbed within 24 hours.

Next are the main points that the teaching of COMP3731/6906 will be based on:

- Lectures will be Asynchronous. Each lecture will include a whole subject and will last as long as the particular subject dictates (not necessarily 75 minutes). The lecture will be captured and published on the course's Brightspace (D2L) shell, timely. You may watch it at your convenience; however, you are strongly advised to follow the outline's schedule.
- Despite the asynchronous nature of lecturing, the total time of instruction will be about 30 hours, which is the normal instruction time for a 3-credit course.
- Lecture notes will be published on D2L. They will consist of:
 - 1. Introduction to Scientific Computing (Power Point presentation (in pdf format))
 - 2. Introduction to Scientific Computing (Main set of notes (instead of textbook))
 - 3. Introduction to MATLAB (Power Point presentation (in pdf format))
- Every week there will be two 75-minute online **Virtual Office Hours** which will take place during Slot 17, TR 09:00-10:15am. Slot 17 is the official time slot for COMP 3731/6906. Please note that, virtual office hours are not replacing lecture hours (lectures will be delivered on videos); therefore, people can drop in and out of the virtual office hours as needed.

Course Schedule (It may need to be slightly modified throughout the semester):

Dates	Topics(s)	
Week 1: Sep 9 – Sep 15	Introduction to Scientific Computing, Floating Point Arithmetic, Errors in	
	Computations	
Week 2: Sep 16 – Sep 22	Floating Point Arithmetic, Errors in Computations	
Week 3: Sep 23 – Sep 29	Vector and Matrix Norms, Stability of Algorithms and Conditioning of	
	Problems	
Week 4: Sep 30 – Oct 6	Stability of Algorithms and Conditioning of Problems, Introduction to MATLAB	
Week 5: Oct 7 – Oct 13	Synthetic Division (Horner's Rule)	
(MIDTERM BREAK -		
Oct 12-13)		
Week 6: Oct 14 – Oct 20	Synthetic Division (Horner's Rule), Catch up or review of some subjects	
Week 7: Oct 21 – Oct 27	(Midterm Exam – Oct 22)	
	Numerical Solution of Nonlinear Equations	
Week 8: Oct 28 – Nov 3	Numerical Solution of Nonlinear Equations	
Week 9: Nov 4 – Nov 10	Concepts of Numerical Linear Algebra, the LU decomposition & Gaussian	
	Elimination (Systems of Linear Equations)	
Week 10: Nov 11 – Nov 17	Concepts of Numerical Linear Algebra, the LU decomposition & Gaussian	
(Remembrance Day	Elimination (Systems of Linear Equations)	
Holiday - No lectures -		
Nov 11)		
Week 11: Nov 18 – Nov 24	Interpolation; Approximation; The Linear Least squares problem	
Week 12: Nov 25 – Dec 1	Numerical Integration	
Week 13: Dec 2 – Dec 4	Numerical Integration	
Final Exam Period: Wednesday, Dec 9 to Friday, Dec 18.		

Assignment Schedule (It may need to be slightly modified throughout the semester):

Assignment #	Assignment Due at 11:59pm NT
1	TBA
2	TBA
3	TBA
4	TBA
5	TBA
6	TBA
7	TBA

Important notes to read, understand and follow for this course:

1. General Notes

- ACADEMIC INTEGRITY (See Regulation 6.12): Within the University community there is a collective responsibility to maintain a high level of scholarly integrity. A student is expected to adhere to those principles which constitute proper academic conduct. Academic misconduct cannot be condoned or even appear to be condoned. A student has the responsibility to know which actions, as described under Academic Offences, could be construed as dishonest or improper.
- Any email messages to the instructor should contain COMP3731 or COMP6906 in the subject line and be sent to george@mun.ca. Messages should be sent from a valid Memorial University account. I will respond ONLY to well thought-out, well-phrased questions, and only to questions that will not require more than a 3 to 4 line answer. If the question requires a long or complicated answer, I will ask you to "see" me during office hours. I will definitely NOT engage into a conversation via email.
- There will be no lectures from Monday, October 12 to Tuesday, October 13 (Midterm Break), and Wednesday, November 11 (Remembrance Day Holiday).
- Thursday, October 15, 2020 will follow **Tuesday's schedule**. Friday, October 16, 2020 will follow **Monday's schedule**.
- The lectures and all material delivered or provided in COMP 3731/6906, including any visual or audio recording thereof, are subject to copyright. It is prohibited to record or copy by any means, in any format, openly or surreptitiously, in whole or in part, in the absence of express written permission from the course instructor (G. Miminis) any of the lectures, materials provided or published in any form during or from the course.

2. Assignments

- There will be given 7 assignments throughout the semester that will involve theory and programming. Programming assignments will be chosen to illustrate the numerical inaccuracies that can appear because of the *finite precision* of computers. Programming assignments should be written in MATLAB, which is a very effective and relatively easy to learn language. MATLAB will be introduced in one of the lectures.
- Assignments should be submitted in pdf format. The title of your submission should have the format: "your name course number assignment number", for example:

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"George Miminis - COMP6906 - Assignment 4"
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If the assignment involves programming in MATLAB as well as mathematical analysis of the implemented problem, then compress the pdf file of your analysis along with the MATLAB code into a zip file and submit the zip file. The title of the zip file as well as the title of the pdf file of your analysis should follow the above mentioned format, that is, "your name - course number - assignment number", the names of the MATLAB files should be "sensible".

Each assignment should be uploaded in the correct format, and in the correct folder, using Brightspace's Dropbox (instructions will be given on the first assignment). Please be aware that the files you submit for evaluation should be uploaded on or before the due date and much before the cut off time, 11:59pm

Newfoundland Time. Even if you are late by a few seconds you will not be allowed to submit your work; hence you should try to upload the files 15 minutes before the cut off time since your system clock is not synchronized with CITL's system clock, which the cutoff time is based on. Please note that if your file has been correctly uploaded, you will get a confirmation receipt from the **Dropbox** tool. If you do not receive this receipt, contact the CITL Support team. Your instructor will not be able to help you in this regard. It is **very important** to remember that what is not uploaded, cannot be marked. It is your responsibility to make sure that the **correct** files are actually uploaded, so please **do** check for the confirmation that your files have been uploaded.

- Note that, while the due times for submissions are at 11:59pm Newfoundland Time, help may not be available after 4:30pm on the due date. The last few hours from 4:30pm 11:59pm should be used to finalize your work and submit it. Any questions you may have about the assignments should be asked well in advance of the due date/time to allow time for help to be given.
- Although I encourage cooperation in understanding and solving the assignments (Please take advantage of my office hours), eventually assignments are to be written INDIVIDUALLY. If plagiarism of ANY kind is detected, the assignment will be given -10 NOT just 0 (Assignments are marked out of 10). Please note that a -10 in an assignment also cancels out another perfect assignment. See the "ACADEMIC INTEGRITY" note above.
- No late submissions will be accepted. If, for special circumstances (such as medical or bereavement), you miss a deadline for a grade item, notify your instructor as soon as possible and not later than 48 hours, providing an explanation for the missed work and any related documentation (if documentation is required). Failure to do this can result in a mark of 0% for that work. Please refer to the **current University policy** regarding medical notes and the information to be in them. For more information, please see the University Calendar University Regulations General Academic Regulations (Undergraduate) **6.7.5 Exemptions from Parts of the Evaluation** and **6.15 Appeal of Decisions** or consult the Registrar's Office. If your reasons for the missed work are acceptable, then your instructor will provide details of any alternate evaluation scheme.
- I am aware of sites that "help" students with assignments. It is not worth using them, I will most probably detect it and I will examine you orally on the details of the solution of the particular assignment. I reserve the right to examine the student orally on the details of a particular assignment if I suspect plagiarism.

3. Exams

• Students will be expected to complete the midterm exam and final exam online in Brightspace (D2L) using the Quiz tool.

• Midterm Exam

- The Midterm exam will be **Semi-Synchronous**. Meaning that, it will take place on **Thursday 9:00am-10:15am (Newfoundland Time), October 22, 2020**. But it will be a **50-minute** test starting any time within the above 75-minute time slot and finishing in 50 minutes, but no later than 10:15am Newfoundland Time. So, the latest you can start and take advantage of the full 50 minutes, is 9:25am.
- O It is important to note that this course does not have an option for writing a deferred Midterm exam. If, for any reason, you miss the Midterm exam, you should contact your instructor right away, giving the reasons for missing the exam, and requesting that the weight of your Midterm exam be added to the weight of your Final exam. If your request is approved by your instructor, then the weight of your Final exam will be 70%, otherwise your Final exam will be worth 40% and you will receive a 0 for the missed Midterm exam.

Final Exam

- The final exam will be scheduled by the **Registrar's Office** for some time during the regular exam period (**Dec 9 Dec 18**). For the exact final exam date and time, check on **Memorial Self-Service**.
- o Requests for any deferred final exam should be made by filling in the Request for Deferred Exam form and submitting it to the head of the Department of Computer Science (or their delegate) and to your instructor. The completed form should be sent to the following email addresses:
 - cs-chair@mun.ca, compsci@mun.ca, george@mun.ca
- o This form can be accessed from: https://www.mun.ca/computerscience/ugrad/Deferred_Exam_Request_Form_20190623.pdf

No supplementary examination will be given for this course.

4. Student support

- Memorial University of Newfoundland is committed to supporting inclusive education based on the
 principles of equity, accessibility and collaboration. Accommodations are provided within the scope of the
 University Policies for the Accommodations for Students with Disabilities
 (www.mun.ca/policy/site/policy.php?id=239). Students who may need an academic accommodation are
 asked to initiate the request with the Glenn Roy Blundon Centre at the earliest opportunity
 (www.mun.ca/blundon).
- Help with any Brightspace (D2L) technical issues is available by contacting the **CITL Support Centre** via phone (1-866-435-1396, or locally at 709-864-8700), online chat (when available) or via their ticketing system. This contact information is available at: https://www.citl.mun.ca/support/
- Please note that Memorial University offers a broad range of supports. For a more comprehensive list of student supports and resources, please check out the following links:
 - o https://www.mun.ca/munup/support/
 - o https://www.mun.ca/main/students.php
 - o https://www.munsu35.ca/resource-centres/

References:

- 1. **G. Miminis, Class notes.**
- 2. G. Dahlquist, A. Bjorck, "Numerical Methods in Scientific Computing, Vol. 1", ISBN 978-0-898716-44-3, SIAM, 2008.
- 3. G. Golub, C. Van Loan, "Matrix Computations", John Hopkins University Press (4th edition) (ISBN 978-1-4214-0794-4), 2013.
- 4. C. Woodford, C. Phillips, "Numerical Methods with Worked Examples", Matlab Edition, 2nd edition, Springer, 2012.
- 5. Bertil Gustafsson, "Fundamentals of Scientific Computing", Springer, 2011.
- 6. Dianne P. O'Leary, "Scientific Computing With Case Studies", SIAM, 2009.
- 7. G. W. Recktenwald, "Numerical Methods with MATLAB: Implementations and Applications", Prentice Hall, 2000.
- 8. D. Kahaner, C. Moler, S. Nash, "Numerical Methods and Software", Prentice-Hall (ISBN 0-13-627258-4), 1989.
- 9. T. Coleman, C. Van Loan, "Handbook for Matrix Computations", SIAM (ISBN 0-89871-227-0), 1987.
- 10. J. Vandergraft, "Introduction to Numerical Computations", Academic Press (ISBN 0-12-711356-8), 1978.