

Fast Methods in Scientific Computing

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- (1). **Meeting times.** TTh 11.00 – 12.30, RLM 12.166.
- (2). **Office hours.** In RLM 11.164: Mondays 13:00 – 14:30. Tuesdays 13:30 – 15:00.
- (3). **Website.** All course material (lecture notes, homeworks, tutorial codes), and an up-to-date timeline will be posted at the following URL:

http://users.ices.utexas.edu/~pgm/Teaching/2019_393C/

- (4). **Course objectives.** The class will describe analysis based computational techniques for rapidly and accurately solving some of the key tasks encountered in scientific computing. We will cover methods for solving equations that arise in molecular biology, radar scattering and medical imaging, electrostatics, astrophysics, mechanical engineering, and many other fields. The equations we study (Laplace, Helmholtz, linear elasticity, Stokes, Maxwell, etc) often form the core of a computational model, and the speed with which they can be solved is often what decides how realistic of a computational model can be used.

The course will also cover a range of topics in numerical linear algebra such as Krylov solvers, randomized algorithms for low-rank approximation, and algorithms for so called “rank-structured” matrices. These techniques are very useful in the study of fast solvers for elliptic PDEs, but have also found plenty of use in data analysis and other applications.

- (5). **Prerequisites.** The course assumes a solid foundation of upper division undergraduate course work on PDEs and numerical analysis. Specific pre-requisite skills include: (1) Familiarity with the Laplace and Helmholtz equations, how they arise in physical applications, well-posedness of boundary value problems, Green identities, etc. (2) Basic numerical analysis concepts such as order of convergence of a numerical method, stability, quadratures, and floating point arithmetic. (3) Very solid understanding of linear algebra and matrix methods, including the SVD, LU, and the QR factorizations, and methods for computing them.

The course will in part discuss Krylov methods for solving linear systems and for finding approximate eigenvalues and eigenvectors of matrices. Some prior familiarity with iterative methods is helpful, however.

Familiarity with basic concepts from probability theory will be useful for the section on randomized algorithms for matrix computations (multivariate normal distributions, the concepts of expectations, co-variance matrices, etc).

Knowledge of basic programming in Matlab is assumed. Students are free to use other programming environments to work examples and to do homeworks, but all tutorial codes and examples covered in class will use the Matlab syntax.

Some familiarity with Fourier methods will be very helpful.

- (6). **Grading.** The final grade will be based on homeworks and a project:

- 50% for homeworks (5 homeworks, each worth 10%).
- 10% for submitting a carefully typed up “reference solution” to one or two homework problems.
- 40% for a final project.

(7). **Text.** The course is defined by the material covered in class, and there is no “official” text book. However, extensive latexed notes will be made available on the course webpage. These notes are new, and comments and suggestions are greatly appreciated. (Mistakes, passages that might be unclear, general suggestions for improvement, . . .)

(8). **Homeworks.** There will be 5 homeworks, with due dates posted on the course webpage.

The homeworks can be done individually or in pairs.

Each individual in the course (not each pair!) will be required to sign up to be responsible for producing “reference solutions” to one or two homework problems. These should be a typed solutions, and should include Matlab codes where appropriate. The instructor will review the submitted reference homework, and suggest edits/corrections where appropriate. Once the reference homework is complete, it will be posted to the course webpage as a solution. You are allowed to collaborate in producing the reference homework if you choose, but only one student will get credit for the problem.

Each regular homework set will be worth 10% of the grade. In addition, your reference homework problem will be worth 10%.

(9). **Project.** Your grade in this course will to 40% be based on a final project. You are allowed (and encouraged!) to work in pairs on the project. Groups of three students could be allowed if the project chosen is particularly labor intensive, but this requires instructor permission.

A number of suggested projects will be listed on the course webpage. You are also very welcome to think of projects on your own; if you want to go with this option, you need to discuss the chosen project with the instructor to get it approved. Please initiate this discussion no later than March 15, if possible.

(10). **Time line.** The plan is to cover the following topics:

<i>Week:</i>	<i>Material covered:</i>
1:	Introduction: Objectives of the course. Quick review of basic elliptic PDEs and their connections to physical applications. Analytic solution formulas, and their relationship to numerical methods. Fast algorithms for global operators.
2:	Linear algebra: Review of basic matrix factorizations. Techniques for computing low-rank approximations to matrices. Randomized methods for matrix computations.
4:	Rank-structured matrices: What they are, where they arise in applications, how they enable fast solvers (and fast matrix algebra more generally).
5:	Krylov methods for solving linear systems and computing partial spectral decompositions.
7:	Fast solvers for elliptic PDEs based on the FFT and related techniques.
8:	Direct solvers for elliptic PDEs based on Gaussian elimination combined with nested dissection ordering of the nodes (“multifrontal methods”). Sweeping solvers.
10:	Boundary integral equations. How a PDE can be rewritten as an integral equation. Advantages and disadvantages. Second kind Fredholm equations. Reduction of dimensionality.
12:	The Fast Multipole Method, and fast summation techniques. The kernel evaluation map. Kernel-independent FMMs and \mathcal{H} -matrices.
14:	Fast direct solvers for integral equations.
15:	(If time permits. . .) Johnson-and-Lindenstrauss theory, and connections to analysis of complex high dimensional data sets.

(11). **This is a new course!** This is the first time this course is run. As a consequence, the timeline given above is just a rough guide — we may find that some topics require more or less time as we go. The course webpage will be updated during the semester to show the actual pace of progress.

Moreover, all homeworks and projects are also mostly new and untested. This means that they might be easier or harder than intended. If something seems odd, then please notify the instructor asap — you might very well have found a mistake!

University Policies:

Academic Integrity. Each student in the course is expected to abide by the University of Texas Honor Code: “As a student of The University of Texas at Austin, I shall abide by the core values of the University and uphold academic integrity.” Plagiarism is taken very seriously at UT. Therefore, if you use words or ideas that are not your own (or that you have used in previous class), you must cite your sources. Otherwise you will be guilty of plagiarism and subject to academic disciplinary action, including failure of the course. You are responsible for understanding UT’s Academic Honesty and the University Honor Code which can be found at the following web address: http://deanofstudents.utexas.edu/sjs/acint_student.php

Q Drop Policy. If you want to drop a class after the 12th class day, you’ll need to execute a Q drop before the Q-drop deadline, which typically occurs near the middle of the semester. Under Texas law, you are only allowed six Q drops while you are in college at any public Texas institution. For more information, see: <http://www.utexas.edu/ugs/csacc/academic/adddrop/qdrop>

University Resources for Students. Your success in this class is important to me. We will all need accommodations because we all learn differently. If there are aspects of this course that prevent you from learning or exclude you, please let me know as soon as possible. Together we’ll develop strategies to meet both your needs and the requirements of the course. There are also a range of resources on campus:

Services for Students with Disabilities: This class respects and welcomes students of all backgrounds, identities, and abilities. If there are circumstances that make our learning environment and activities difficult, if you have medical information that you need to share with me, or if you need specific arrangements in case the building needs to be evacuated, please let me know. I am committed to creating an effective learning environment for all students, but I can only do so if you discuss your needs with me as early as possible. I promise to maintain the confidentiality of these discussions. If appropriate, also contact Services for Students with Disabilities, 512-471-6259 (voice) or 1-866-329- 3986 (video phone). <http://ddce.utexas.edu/disability/about/>

Counseling and Mental Health Center: Do your best to maintain a healthy lifestyle this semester by eating well, exercising, avoiding drugs and alcohol, getting enough sleep and taking some time to relax. This will help you achieve your goals and cope with stress.

All of us benefit from support during times of struggle. You are not alone. There are many helpful resources available on campus and an important part of the college experience is learning how to ask for help. Asking for support sooner rather than later is often helpful.

If you or anyone you know experiences any academic stress, difficult life events, or feelings like anxiety or depression, we strongly encourage you to seek support.

<http://www.cmhc.utexas.edu/individualcounseling.html>

Libraries: <http://www.lib.utexas.edu/>

ITS: <http://www.utexas.edu/its/>

Student Emergency Services: <http://deanofstudents.utexas.edu/emergency/>

BeVocal: BeVocal is a university-wide initiative to promote the idea that individual Longhorns have the power to prevent high-risk behavior and harm. At UT Austin all Longhorns have the power to intervene and reduce harm. To learn more about BeVocal and how you can help to build a culture of care on campus, go to: <http://wellnessnetwork.utexas.edu/BeVocal>

Important Safety Information: If you have concerns about the safety or behavior of fellow students, TAs or Professors, call BCAL (the Behavior Concerns Advice Line): 512-232-5050. Your call can be anonymous. If something doesn't feel right — it probably isn't. Trust your instincts and share your concerns.

The following recommendations regarding emergency evacuation from the Office of Campus Safety and Security, 512-471-5767, <http://www.utexas.edu/safety/> Occupants of buildings on The University of Texas at Austin campus are required to evacuate buildings when a fire alarm is activated. Alarm activation or announcement requires exiting and assembling outside.

- Familiarize yourself with all exit doors of each classroom and building you may occupy. Remember that the nearest exit door may not be the one you used when entering the building.
- Students requiring assistance in evacuation shall inform their instructor in writing during the first week of class.
- In the event of an evacuation, follow the instruction of faculty or class instructors. Do not re-enter a building unless given instructions by the following: Austin Fire Department, The University of Texas at Austin Police Department, or Fire Prevention Services office.
- Link to information regarding emergency evacuation routes and emergency procedures can be found at: www.utexas.edu/emergency

Title IX Reporting. Title IX is a federal law that protects against sex and gender based discrimination, sexual harassment, sexual assault, sexual misconduct, dating/domestic violence and stalking at federally funded educational institutions. UT Austin is committed to fostering a learning and working environment free from discrimination in all its forms. When sexual misconduct occurs in our community, the university can:

- (1) Intervene to prevent harmful behavior from continuing or escalating.
- (2) Provide support and remedies to students and employees who have experienced harm or have become involved in a Title IX investigation.
- (3) Investigate and discipline violations of the university's relevant policies.

Faculty members and certain staff members are considered "Responsible Employees" or "Mandatory Reporters," which means that they are required to report violations of Title IX to the Title IX Coordinator. I am a Responsible Employee and must report any Title IX related incidents that are disclosed in writing, discussion, or one-on-one. Before talking with me, or with any faculty or staff member about a Title IX related incident, be sure to ask whether they are a responsible employee. If you want to speak with someone for support or remedies without making an official report to the university, email advocate@austin.utexas.edu For more information about reporting options and resources, visit titleix.utexas.edu or contact the Title IX Office at titleix@austin.utexas.edu

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Religious holidays. If you plan to miss class due to observance of a religious holiday, please let me know *at least two weeks in advance*. You will not be penalized for this absence, although you will still be responsible for any work you will miss on that day if applicable. Check with instructor for details or arrangements.